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Chemical education at the high school: Survey of students' conceptions on bonding and design of a didactic sequence on the notion of bonding

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Indice

Purpose of the thesis work	5
 Chapter 1 - What is the health state of chemistry teaching and learning in Italy?	
Introduction	6
1.1 Objectives of the test	7
1.2 Analysis and discussion of the results	8
1.3 Conclusions	41
References	45
 Chapter 2 - Educational research on the concept of interatomic bonding: state of the art and theoretical premises for the development of a didactic sequence	
Introduction	47
2.1 Some methodological notes	48
2.2 Theoretical conceptual framework related to the teaching of the concept of interatomic bonding	52
2.3 Strategies and precautions for teaching and learning interatomic bonding	54
2.4 Cognitive/pedagogical aspects	64
2.5 Alternative conceptions	68
2.6 Lexical choices in the didactic transposition of the interatomic bonding	75
2.7 Conclusions	77
References	80
 Chapter 3 - Historical-epistemological evolution of the concept of interatomic bonding	
Introduction	83
3.1 Historical-epistemological evolution of the concept of interatomic bonding	85
3.1.1 The notion of valence	86
3.1.2 The notion of chemical affinity	87
3.1.3 The electric properties of matter, Berzelius' dualistic theory and the origin of the electronegativity notion	88
3.1.4 Beyond Berzelius, new perspectives on chemical bonding	90
3.1.5 Atomic structure models	93
3.1.6 Electrical theory of bonding	94
3.1.7 Lewis-Langmuir theory of bonding	97
3.2 Conclusions	104
References	107
 Chapter 4 - A teaching sequence on the concept of interatomic bonding	
Introduction	109
4.1 Detection of students' initial conceptions and preliminary activities	114
4.2 London dispersion forces	117
4.3 Covalent bonding model	142
4.4 Dipole-dipole bonding and hydrogen bridge bonding	182
4.5 Ionic bonding model	202
4.6 Metallic bonding mode	223
4.7 Conclusive summary activity	241
References	248

Chapter 5 - Experimentation of the didactic sequence in the classroom. Concluding remarks.

5.1 Context choice and work sheets selection	250
5.2 Procedure for data collection	251
5.3 Results of the experimentation	251
5.4 Concluding remarks	268
References	273
Appendix 1	274
Acknowledgements	279

Purpose of the thesis work

Interatomic bonding is a crucial notion in chemistry and a challenge for chemical education. Educational research shows that secondary school students develop a number of alternative conceptions related to interatomic bonding. The difficulty of this topic is related to several issues, such as:

- i) the need for a range of different models, that has to be properly justified;
- ii) the limited comprehension of models and their use by students. In fact, a reflection on the nature of models, their purpose and their relationship with the physical realm is often disregarded by teachers and textbooks;
- iii) the continuous transition between macroscopic, microscopic and symbolic levels that is not always pointed out by teachers;
- iv) the lack of a unifying conceptual frame for the treatment of interatomic bonding. In fact, student often perceive intra- and inter-molecular bonding as radically distinct phenomena and they do not realize the common electrostatic nature of all kinds of interatomic bonds.

In this context, the main purpose of the present thesis work was to design a teaching sequence on the notion of interatomic bonding for high school students. Our sequence tries to overcome some of the problems related with this concept, which are extensively denounced by the literature.

The significance of building a didactic sequence, and to produce a concrete operational tool to be made available to high school teachers, lies in the need to bridge the gap existing between educational research and daily teaching practices.

This thesis work is part of a research stream that seek new strategies and solutions for overcoming learning obstacles and contrasting the spread of alternative conceptions on interatomic bonding.

This thesis work was carried out through the following actions:

- Design of questionnaires to be administered to high school students, aimed at detecting misconceptions related with the notion of interatomic bonding and other basic chemical concepts.
- Bibliographic survey of the international literature currently available on the notion of interatomic bonding and its didactic transposition.
- Analysis of the historical-epistemological evolution of the concept of interatomic bonding, in order to highlight epistemological issues relevant to the teaching of this notion.
- Design of a teaching sequence on the notion of interatomic bonding to be administered to first- and second-year high school students.
- Experimentation of the teaching sequence in a second class of a technical school and analysis of results.

The present manuscript is structured as follows:

- Chapter 1 - What is the health state of chemistry teaching and learning in Italy?
- Chapter 2 - Educational research on the concept of interatomic bonding: state of the art and theoretical premises for the development of a didactic sequence
- Chapter 3 - Historical-epistemological evolution of the concept of interatomic bonding
- Chapter 4 - A teaching sequence on the concept of interatomic bonding
- Chapter 5 - Experimentation of the didactic sequence in the classroom. Concluding remarks.

Chapter 1

What is the health state of chemistry teaching and learning in Italy?

Introduction

The intrinsic complexity of chemical concepts, due to their high degree of abstractness and the essential need to make the transition between the three explanatory levels of chemistry (the macroscopic, the microscopic and the symbolic), is a relevant learning obstacle, which fosters the raise of several misconceptions. Several studies denounce students' difficulties to achieve a meaningful learning of chemical notions: these difficulties seem to persist over time and in different cultural contexts (Fang et al. 2014; Mayer 2011; Nakhleh 1992; Othman et al. 2008; Taber et al. 2012; Ünal et al. 2006). The Italian secondary school makes no exception: OCSE-PISA data show that the average level of scientific culture of Italian students is lower as compared to other countries (Cardellini 2004). In fact, several studies carried out in the Italian context, aimed at evaluating the effectiveness of scientific (namely, chemistry) teaching testify to the inadequate level of understanding and the massive presence of misconceptions. All this raises questions on the adequacy and effectiveness of the chemistry teaching-learning process. For example, surveys on foundational scientific concepts such as physical states of matter and physical transformations (Carrozza 2005), carried out over several years at Italians Technological and Scientific High Schools, highlights criticalities deriving from transmissive teaching approaches, which fail to underline the relationships between scientific concepts and phenomena belonging to everyday contexts. As a result, students prove unable to contextualize their knowledge in real life situations. Roletto et al. (2003) detect misunderstanding of the concept of mole among students of advanced classes of technical or scientific high schools. Most interestingly, Mirone and Roletto (1999) found these very same problems in university freshmen of the Chemistry and Industrial Chemistry courses. The two authors ascribe these problems to inadequate teaching practices:

“Most students coming out from Italian secondary schools do not master sufficiently the concept of chemical substance and have confused ideas about the distinctions between simple substances and compounds, between homogeneous and heterogeneous mixtures, between chemical reactions and other transformations of matter. These difficulties partially derive from the fact that, *in our schools, chemistry is taught in a predominantly theoretical (not to say bookish) way*, which inevitably leads to privilege the submicroscopic level of atoms and molecules and *to overshadow the level of observable phenomena* ” (Mirone e Roletto 1999, our translation, italics added).

Other surveys conducted on university freshmen indicate that a significant fraction of students did not understand the distinction between atom and molecule in an operational way (Rihab and Cardellini 2011) and show the necessity to improve the meaningful learning of foundational thermodynamics concepts (Mirone and Benedetti 2001).

The above mentioned surveys carried out in the Italian context over a period of almost 20 years showed that the outcomes of chemistry teaching practices in upper secondary school are largely unsatisfactory. In order to acquire more recent data on the level of understanding of basic chemical concepts by secondary school students, we designed a test that was administered to students of the terminal classes of Scientific High School (Liceo Scientifico tradizionale e Opzione Scienze Applicate). The test allowed probing the level of chemical knowledge and competences possessed by students who are about to leave upper secondary school cycle and enter University.

1.1. Objectives of the test

The questionnaire focuses on some conceptual knots of chemistry and was designed in order to assess the level of chemical knowledge acquired by students leaving secondary school, and to compare them with those expected for freshmen who enter scientific university courses.

More in detail, this series of 18 questions aims assessing the level of understanding of some basic general chemistry concepts and to highlight the presence of misconceptions, if any. The test contains various question types, with different mode of answers (written texts, sketches, multiple choices, etc.) aimed at getting information on students' meta-cognitive processes. For example, the answers involving iconic representations allow, better than a written text, to check the reasoning patterns and mental models of students, and to clarify their level of effective understanding. Here is a brief description of the concepts addressed by the test.

The first question concerns the meaning and representation of a model. The second concerns the particle representation of matter¹ and the concept of physical state. The third, connected to the second, verifies a competence: the student's ability to apply the ideal gas model to a real context. The fourth question investigates the understanding of the notions of simple substances, compounds, pure substance and mixture, by using iconic representations. The fifth question aims at evaluating the understanding of the atomic shell model, by proposing its application to familiar situations. The next question still concerns the use of the particle model and its representations to identify a pure substance and a mixture, both in the liquid state. Question 7 concerns the notions of intensive and extensive quantity, and its application to everyday-life case. Questions 8 to 10 focus on the themes of chemical and physical transformations, either from a theoretical, iconic or symbolic viewpoint. Questions 11 and 13 investigate the understanding of the concept of mole and its applications in theoretical contexts (stoichiometric ratios in a chemical reaction) and in familiar macroscopic contexts. Question 12 focuses on deciphering symbolic language and the meaning of subscripts in brute formulas. The ability to classify the different types of chemical reactions is explored in question 14. Question 15 is about interatomic (intra or intermolecular) bonding models. Questions 16 and 17 deal with the notions of concentration and dilution. Finally, the eighteenth question deals with what is classified in the periodic table of elements.

The test was administered to 105 students (5 classes) from two different high schools in the Marche region of Italy. The test was administered in paper form to 34 students of the Scientific High School "E. Medi" of Senigallia (AN) on 20 October 2020. The remaining 71 students, from the Scientific and Musical High School "G. Marconi" in Pesaro (PU), took the online test on 25 November 2020 (via the Google Classroom Suite platform) due to the closure of upper secondary schools for the ongoing health emergency. The test was, in all cases, strictly anonymous. Before its administration, the test was shared with the referent teachers of the respective schools, in order to verify their consistency with the contents dealt with by their classrooms.

¹ We refer here to the microscopic model of the structure of matter in which particles, represented by iconic symbols, are endowed with the following properties: indivisibility, non-deformability, invariance of volume and mass. Iconic representations of the model need to take these properties into account and to ensure consistency between the macroscopic properties of the system and their interpretations in terms of particles.

1.2. Analysis of results and discussion

In this paragraph, for each question, the statistical results and meta-cognitive information emerging from the analysis of the acquired answers will be presented in detail.

Question 1: Understanding of the concepts of model, atom, molecule, elementary substance and compound.

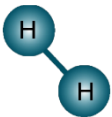
Look at these two images			
$\text{H}-\text{H}$			
In your opinion they represent:			
	YES	NO	I can not answer
The same object			
Different objects			
An atom			
A molecule			
A compound			
Two models of the same molecule			

Figure 1.1 reports the collected results.

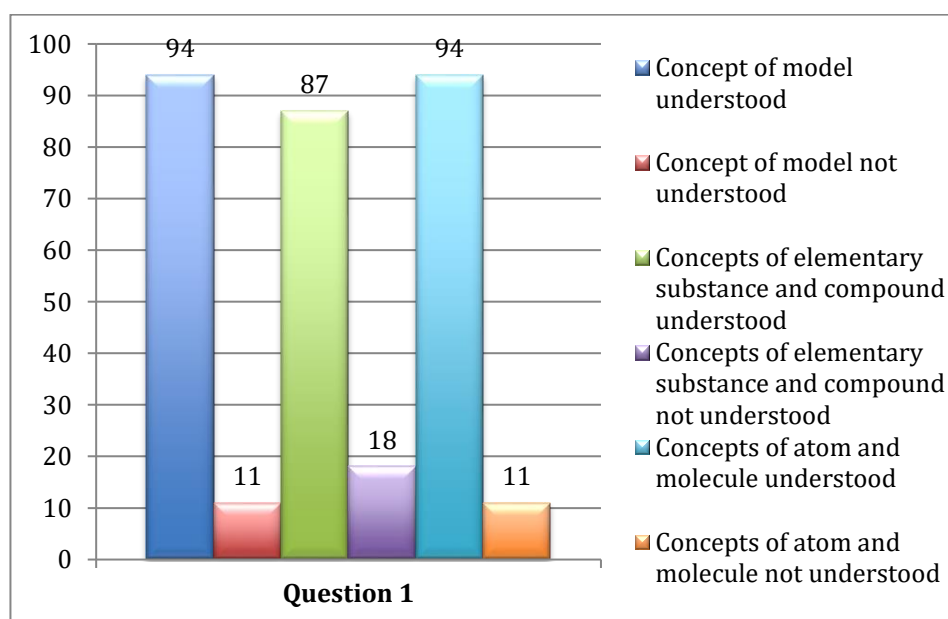


Figure 1.1 Outcomes of the answers to question 1

The correct answers are in order: Yes; No; No; Yes; No; Yes. 94 out of 105 students (89.5%) and 87 out of 105 students (82.9%) correctly recognized the objects represented and were able to distinguish between atom

and molecule, and between elementary substance and compound. 89.5% of the population stated that the representations refer to two models of the same molecule. No justification was required for these answers. The high percentage of correct answers suggests an excellent level of understanding of the concept of model by the students. However, these outcomes need to be examined in conjunction with further questions related to the same or similar subjects.

Question 2: *Particle representation of a gaseous substance before and after compression. Physical states of matter.*

Cars can run on methane, which at ambient T and P is a gas. Methane used as a fuel in cars is stored in tanks under pressure.

Represents methane at the particle level before and after compression:



methane before compression	methane after compression

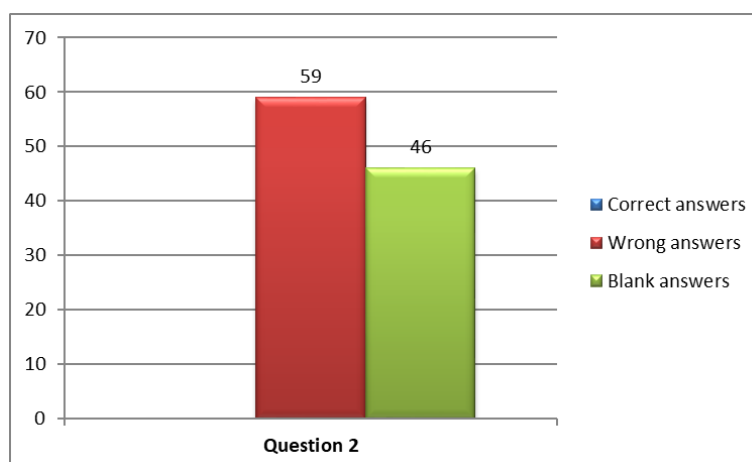


Figure 1.2 Outcomes of the answers to question 2

The question involved the use of the particle model and its representations, in relation to the gaseous state. Acceptable representations had to comply with the following aspects: i) the gaseous state of methane in ordinary conditions (particles represented in a disordered way and far from each other; the distance between particles should be greater than the particle size); ii) the preservation of the substance identity (use of the same symbol for each particles in both boxes); iii) mass conservation (same number of particles in both boxes); iv) volume reduction (particles should be closer to each other in the second box than in the first). None of the 105 students was able to offer a fully correct representation of methane, at the particle level, before and after compression. As many as 46 students (almost 44% of the sample) left the question blank. Figure 1.3 reports some representations² which, although not correct, approach the expected answer. All the representations in figure 1.3 show that the students understood that compression involves a decrease in the distance between

² The representations shown in figures 3 and 4 are the original ones developed by the students: the different formatting of the texts and images is due to the fact that part of the students took the test in paper form and part in online mode

particles. However, these same representations contain inconsistencies that denounce the students' lack of habit to use particle representations.

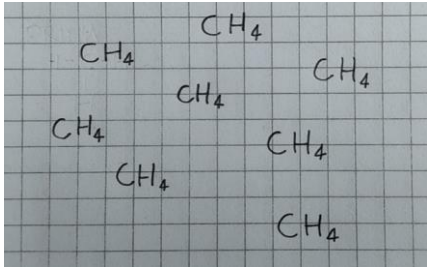
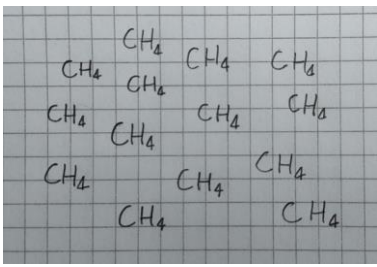
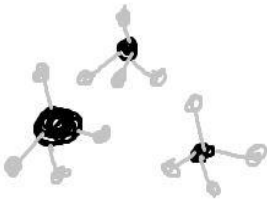
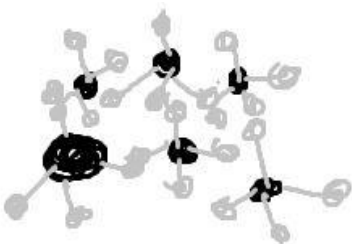
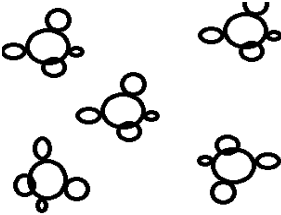
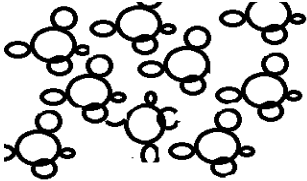
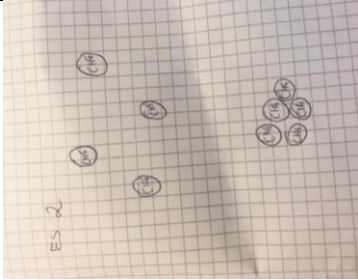
	methane before compression	methane after compression
Student 104		
Student 71		
Student 47		
Student 64		
Student 45		

Figure 1.3 Particle representations provided by students 104-71-47-64-45, respectively

The main problems encountered are:

- No attention is paid to aspects of the model, such as the preservation of particle shape, size or number in the two panels.
- Many representations of the gas after compression show the particles in mutual contact, as they would be in a condensed state. The image of the methane tank might have led students to assume a transition to the liquid state, involved by compression.

Similar findings have been reported by Rihab and Cardellini (2011), authors of a survey similar to ours: “Attributes such as regularity and conservation of particles were ignored by students in over 50% of the examples used in the tests. A misconception that results in many studies is the increase in the size of atoms in the transition from the liquid to the gaseous state”. These problems suggest that particle representations of matter are not exploited by students as reasoning tools. In addition, they do not seem acquainted with their character of model representations, subjected to precise rules and conventions. The question is especially relevant when we consider the extensive use of particle representations made by textbooks.

Another interesting aspect is illustrated by the answer of student 71, who employs symbolic instead of iconic representations. This same behavior was common to many other students. Seemingly, students 47 and 64 recur to stick-and-ball or space-filled structural representations. Although structural aspects are not relevant to this question, their use is probably automatic at the high school level. Finally, student 45 mixes up particle and symbolic representations in a single sign, by drawing a circle with the brute formula of methane inside; more interestingly, he represents a gas-liquid transition instead of a simple compression. These examples, selected from the best representations provided, suggest a poor level of understanding of the particle model of matter and the students' unfamiliarity with its practical use. This is a problem as the understanding of the particle model is essential for the understanding of many basic concepts of chemistry:

“Students of all ages seem to have trouble in understanding and using the scientifically accepted model that matter is made of discrete particles that are in constant motion and have empty space between them. Indeed, *an acceptable concept of the particulate nature of matter lays the foundation for understanding many chemical concepts*: chemical reactions; the effects of pressure, volume, and temperature on gases; changes in state; dissolving; and equilibrium. Unfortunately, many students from all age groups appear to view matter as being made of a continuous medium that is static and space-filling.” (Nakhleh 1992, italics added)

It is also reported (Othman et al. 2008) that poor understanding of the particle structure of matter affects the comprehension of chemical bonding. This suggests that an adequate amount of time should be spent in clarifying the implications of the particle structure of matter and the correct formulation and use of the particle model of matter; moreover, a recursive discussion and deepening of this model is recommendable, in order to reinforce its application and its comprehension, according to the principle of recursive learning of concepts. In this regard, it is worth mentioning an Italian (negative) specificity: the subject of ‘science teaching’ at Scientific High Schools (Liceo Scientifico), that includes several topics (e.g. chemistry, biology, astronomy, geology) is often assigned to teachers without a deep chemistry background. Therefore, it is presumable that teachers do not fully grasp the explanatory power and the formative value of the particle model: this may concur in generating unsatisfactory learning outcomes. A careful study by Vanessa Kind discusses the repercussions on the quality of chemistry learning when chemistry is taught by non-specialists:

“Biologists demonstrated *statistically significantly weaker understanding than chemists and physicists in Chemical bonding*, Mole calculations and Combustion reactions [...] The findings suggest that non-

chemists' content knowledge is insufficient for teaching these chemistry concepts in high schools, despite their possession of 'good' Bachelor of Science degrees" (Kind 2014).

Despite their being referred to science graduates from the United Kingdom, similar conclusions may apply to the Italian context.

Other kind of problems are highlighted by the representations shown in Figure 1.4.

	methane before compression	methane after compression
Student 96	$ \begin{array}{ccc} & H & \\ & & H \\ & C & \\ & & \\ H & & H \end{array} $	$ \begin{array}{ccc} & H & H \\ & C & \\ & H & H \end{array} $
Student 83	H ₂	H ₂ PIU' VICINI DI MOLTO (H ₂ MUCH MUCH CLOSER)
Student 69	$ \begin{array}{cccccccccccc} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ & & & & & & & & & & & \\ & & \cdot & & \cdot & & \cdot & & \cdot & & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{array} $	$ \begin{array}{cccccccccccc} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{array} $
Student 57	particelle meno compatte (less compact particles)	particelle più compatte (more compact particles)
Student 44	CH ₄	CO ₂ +H ₂ O

Figure 1.4 Particle representations provided by students 96-83-69-57-44 respectively

The first representation highlights several alternative conceptions, that are rather serious. Student 96 represents methane through a single particle and associates compression with a decrease in the molecular volume of the methane particle (although he/she does not indicate interatomic bonds between C and H): this denounces confusion between macroscopic and microscopic properties and the misunderstanding of the link between material system and model. This student seems to have understood neither the concept of molecule nor the fact that a physical transformation preserves molecules (in all their aspects) and affects the relationships between molecules. Furthermore, this student has clearly not grasped the difference between intramolecular and intermolecular bonding. Student 83 sketches a single particle and, in addition, he confuses methane with hydrogen. Representation of student 69 is somehow unusual, as molecules are represented by dots: the gaseous state is sketched as an extremely ordered system which, after compression, recalls the layers of a reticular solid. Student 57 describes the transformation verbally, instead of representing it: nevertheless, the verbal description is consistent. The next representation is not a particle representation; it also denounces confusion between physical and chemical transformations. This is surprising as both kind of transformations are discussed in multiple disciplinary contexts (biochemical, geological, etc.): a student in its terminal class is expected to have learnt these notions.

Question 3: Assessment of a competence: application of the law of ideal gases to a real context

Can you explain why tire specialists recommend keeping tire pressure slightly lower in summer as compared to winter?

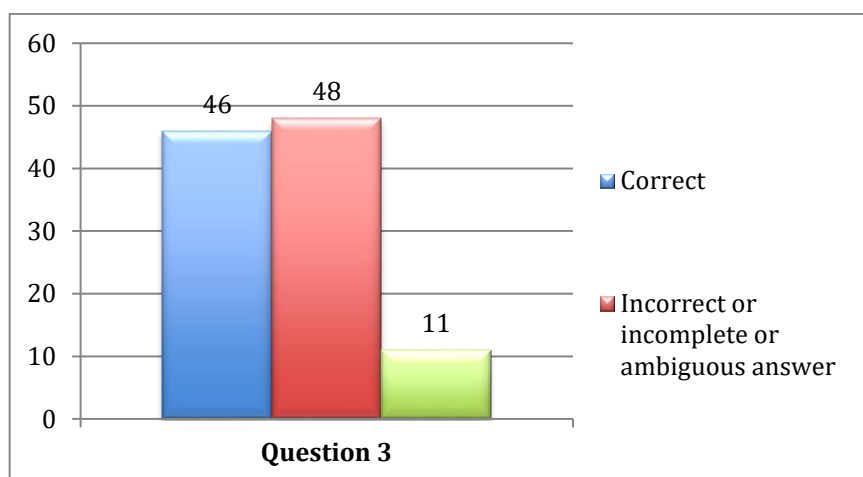


Figure 1.5. Outcomes of the answers to question 3

46 out of 105 students (43.8%) show a good level of understanding of the ideal gas law and the ability to contextualize it in a real context. Some of them argue coherently, by correlating the increase of temperature at constant volume with the increase of pressure. Here are some examples of correct answers given by students.

Student	Answer provided
8	Perché l'aumento di temperatura a volume costante porta ad un aumento di pressione, la quale potrebbe far scoppiare la gomma. (Because the temperature increase at constant volume leads to a pressure increase, which could cause the tire to burst).
58	PERCHE' D'ESTATE LA TEMPERATURA E' MAGGIORE E QUINDI ANCHE LA PRESSIONE AUMENTA IN QUANTO IL RAPPORTO PV/T DEVE ESSERE COSTANTE E, ESSENDO IL VOLUME DI UNO PNEUMATICO SEMPRE LO STESSO ABBIAMO CHE P/T E' COSTANTE. (BECAUSE IN SUMMER THE TEMPERATURE IS HIGHER AND SO THE PRESSURE INCREASES AS THE PV/T RATIO MUST BE CONSTANT AND, BEING THE VOLUME OF A TIRE, ALWAYS THE SAME, WE HAVE THAT P/T IS CONSTANT).
64	Perché pressione e temperatura concorrono in maniera direttamente proporzionale alla forza esercitata sulla superficie della gomma. Siccome in estate aumenta la temperatura è meglio abbassare la pressione per non rischiare di rompere la ruota. (Because pressure and temperature contribute in direct proportion to the force exerted on the surface of the tire. As the temperature increases in summer, it is better to lower the pressure so as not to risk breaking the wheel).
99	PUO' ESSERE SPIEGATO ATTRAVERSO LA SECONDA LEGGE DI GAY LUSSAC CHE AFFERMA CHE A VOLUME COSTANTE, PRESSIONE E TEMPERATURA SONO DIRETTAMENTE PROPORZIONALI. (IT CAN BE EXPLAINED THROUGH THE SECOND LAW OF GAY LUSSAC WHICH STATES THAT AT CONSTANT VOLUME, PRESSURE AND TEMPERATURE ARE DIRECTLY PROPORTIONAL).

Table 1.1 Examples of correct answers to question 3

Other students, while providing substantially correct answers, argue less precisely: they recognize the inversely proportional relationship between volume and pressure, but cannot properly identify the conditions which the question refers to (expansion of a gas at constant volume – pressure increase in the tire).

48 out of 105 pupils (45.7%) provided answers that were either incomplete or ambiguous or completely meaningless, proving the lack of skills required to interpret this phenomenon. Among them, many of them refer to the increase of the tire volume rather than to the pressure increase, as a result of temperature increase. Table 1.2 shows some examples of incorrect or irrelevant answers:

Student	Answer provided
40	Perché a causa del calore la gomma si espande. (Because the tire expands due to the heat).
48	LA PRESSIONE DEI PNEUMATICI IN ESTATE AUMENTA PERCHE' CON IL CALORE QUEST'ULTIMI SI DILATANO PROVOCANDO QUINDI UN INNALZAMENTO DI PRESSIONE E PER MANTENERLI IN UNA GIUSTA PRESSIONE, I GOMMISTI TENTANO A SGONFIARE LIEVEMENTE LO PNEUMATICO. (THE PRESSURE OF TIRES INCREASES IN SUMMER BECAUSE WITH THE HEAT THE TIRES EXPAND, THUS CAUSING A PRESSURE INCREASE AND TO KEEP THEM IN THE RIGHT PRESSURE, THE TIRE SPECIALISTS TRY TO SLIGHTLY DEFLATE THE TIRE).
63	Perché d'estate è più caldo e quindi aumenta l'agitazione degli atomi e quindi aumenta il volume. (Because in summer it is hotter and therefore atoms' agitation increases and therefore the volume increases).
68	Perché con il calore aumenta il volume del gas e la gomma potrebbe scoppiare. (Because with the heat the gas volume increases and the tire might burst).
44	PERCHE' ALL'INTERNO DEGLI PNEUMATICI NEL PERIODO ESTIVO CON IL CALORE AUMENTA IL MOVIMENTO DELLE PARTICELLE PRESENTI AL SUO INTERNO. (BECAUSE INSIDE THE TIRES, IN THE SUMMER PERIOD, THE MOVEMENT OF THE PARTICLES FOUND INSIDE IT INCREASES WITH HEAT).
46	PERCHE' LA TEMPERATURA AMBIENTALE INFLUISCE SULLA PRESSIONE DELLE GOMME, QUINDI IN ESTATE LA PRESSIONE EFFETTIVA SARA' LEGGERMENTE PIU' ALTA DI QUELLA REGISTRATA. (BECAUSE THE ENVIRONMENTAL TEMPERATURE AFFECTS TIRES' PRESSURE, SO IN THE SUMMER THE ACTUAL PRESSURE WILL BE SLIGHTLY HIGHER THAN THAT RECORDED).
85	PERCHE' LA PRESSIONE POTREBBE AUMENTARE CON LA TEMPERATURA. (BECAUSE PRESSURE MIGHT INCREASE WITH TEMPERATURE).
62	PERCHE' IL CALORE ALLONTANA GLI ATOMI DEL GAS CHE E' ALL'INTERNO DELLE GOMME QUINDI CONVIENE MANTENERE UNA PRESSIONE PIU' BASSA. (BECAUSE HEAT MOVES AWAY THE ATOMS OF THE GAS INSIDE THE TIRES SO IT IS CONVENIENT TO MAINTAIN A LOWER PRESSURE).
41	SE SONO TROPPO GONFIE HANNO MENO GRIP IN CURVA E FRENATA. (IF THEY ARE TOO SWELLED, THEY HAVE LESS GRIP IN TURNING AND BRAKING).
86	Poiché in estate si tendono a fare più km in auto e soprattutto perché le alte temperature e l'asfalto molto caldo potrebbero andarle a usurare o anche a scoppiare. (Because in summer people tend to drive more kilometers and above all because the high temperatures and very hot asphalt could wear them out or make them burst).

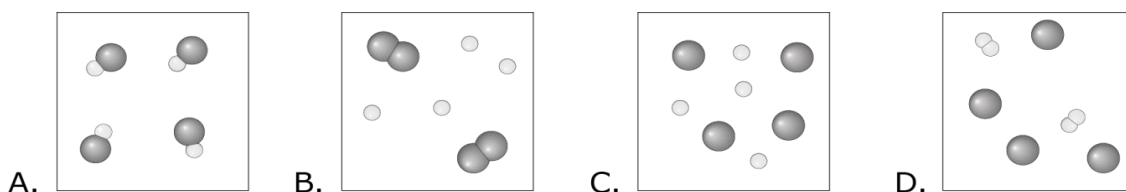
Table 1.2 Examples of incorrect or incomplete answers to question 3

Finally 11 students (10.5%) did not answer. The fact that such a high percentage of students has not been able to provide adequate answers suggest the tendency to mnemonic learning (induced by transmissive teaching practices), which does not stimulate reasoning and does not contextualize theoretical knowledge in the real world. Carrozza (2005) interestingly remarks that: "Very often, phenomena investigated during laboratory activities are not related to phenomena detectable in the material realm around us". Similarly, Mirone and Benedetti (2001) remark: "Improvement is possible on condition that students are trained by their teachers to

face problems related with new situations or known (situations) considered from new viewpoints – that can be dealt with the knowledge that students already possess". This is the right way for fostering the development of new skills: "Students should be actively encouraged to extend their knowledge beyond the area in which it was built" (Bodner 1991, cited in Mirone e Benedetti 2001).

Question 4: *Understanding the distinction between simple substance and compound, substance and mixture of substances, physical states and particle model of matter.*

Look at the following particle representations of different systems. Associate each drawing with the caption that seems most appropriate to you (more alternatives are possible for the same drawing)



	Corresponding letter (s)
A compound	
Mixture of two elementary (or simple) substances	
Mixture of compounds	
Mixture of two monoatomic substances	
Mixture of a compound and an elementary (or simple) substance	
A gaseous substance	
Mixture of a monatomic substance and a diatomic substance	

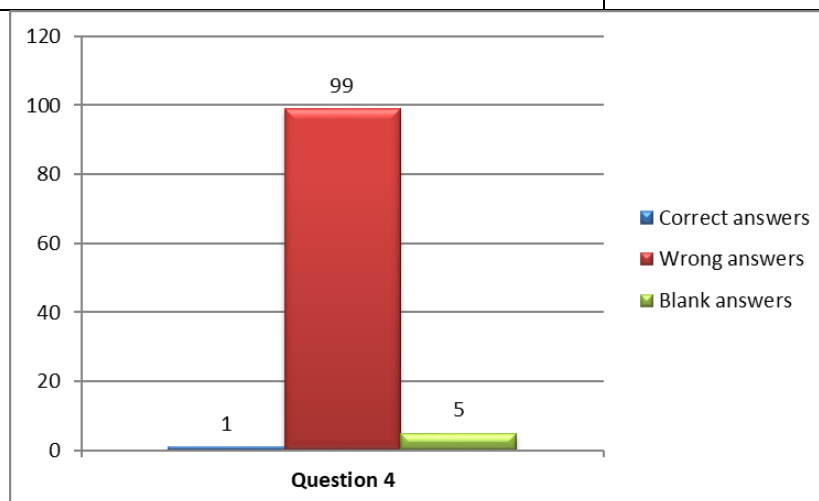


Figure 1.6 Outcomes of the answers to question 4

This question focused on the use of particle representations of matter, that are widely used in textbooks. Students were required to associate each representation with the correct caption, recognizing simple substances and compounds, substances and mixtures, monoatomic and polyatomic substances. The expected answers are, respectively: A; B, C and D; none; C; none; A; B and D. Only 1 student out of 105 provided a fully correct answer, 5 students did not answer, the remaining 99 students provided incorrect and /or contradictory answers, associating incompatible definitions to the same particle representation. As an example, we report the answer of student 81 and compare it with the expected answers:

	Answers provided by student n° 81	Answers expected
	Corresponding letter (s)	Corresponding letter (s)
A compound	A	A
Mixture of two elementary (or simple) substances	D, B	B-C-D
Mixture of compounds	A	-
Mixture of two monoatomic substances	A,B	C
Mixture of a compound and an elementary (or simple) substance	A	-
A gaseous substance	C	A
Mixture of a monatomic substance and a diatomic substance	D	B-D

Table 1.3 Student's answer n° 81 to question 4

Student 81 associated representation A with 4 incompatible definitions, namely a compound and 3 different mixtures. Another inconsistency concerns the double attribution of A to monoatomic substances and compounds. The recognition of a pure gaseous substance proved problematic to many students: 15 students, by neglecting the difference between substance and mixture, associated this option with all panels, while most of them, 61 students, provided answer C. This occurred also with those who formerly recognized A as a compound. The impressive percentage of wrong answers denounces two distinct types of problems: i) students' unfamiliarity with particle representations of matter; ii) the lack of understanding of the difference between substances and mixtures. This difficulty is also denounced by the literature (Cokelez e Dumon 2005). Regarding the differentiation between simple substance and compound, it is significant that many students who got it wrong, had provided correct answer to question 1, which dealt with the same concept. Possibly, the employed terminology was not entirely familiar to students (some may have learnt to designate simple substances as elements). Furthermore, the presence of distractors increased the level of difficulty. It is significant that a survey conducted in 1998 to verify the understanding of some basic concepts of chemistry by freshmen of Chemistry and Industrial Chemistry reports similar difficulties in understanding the concepts of simple substance and compound (Mirone e Roletto 1999). In that study, 19% of the students identified box a of figure 1.7 as "a compound", while 39% of the students designated boxes c and d as "mixtures of compounds". Only 10% of this students' sample was able to provide the right answer.

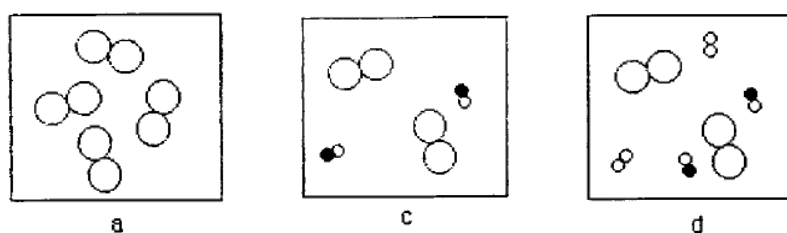


Figure 1.7 3 out of 6 boxes related to a question on the concepts of simple substance and compound (Mirone e Roletto 1999)

According to the authors of this study, in students' minds, the term "compound" undergoes "a shift from the macroscopic level of chemistry (substance made up of different elements) to the microscopic level (molecule composed of several atoms, even identical)" (Mirone e Roletto 1999).

Question 5: Understanding the atomic shell model. Application of concepts to a real context.



Typical red/yellow luminous signs exploit neon lamps.

Neon lamps consist of a glass tube filled with low pressure neon gas. When an electrical discharge passes through the gas, light is emitted.

Specify whether the following statements are true or false:

	TRUE	FALSE
When neon is crossed by the electric discharge, an absorption of energy occurs which allows the electrons to migrate from a lower energy level to a higher one		
The light emitted by neon atoms is not related to specific wavelengths: therefore the specific red / yellow color is observed		
After being excited, electrons release the energy excess in the form of red light and return to the initial energy level		
When electrons of the neon gas atoms absorb energy they shift from an excited energetic state to a fundamental one		
Colored light emission in fireworks is based on a similar phenomenon as that occurring in a neon lamp		

This question consists of 5 statements related to the atomic shell model; the student had to decide whether they were true or false. The expected answers are, respectively: TRUE; FALSE; TRUE; FALSE; TRUE. The graph in figure 1.8 shows the results:

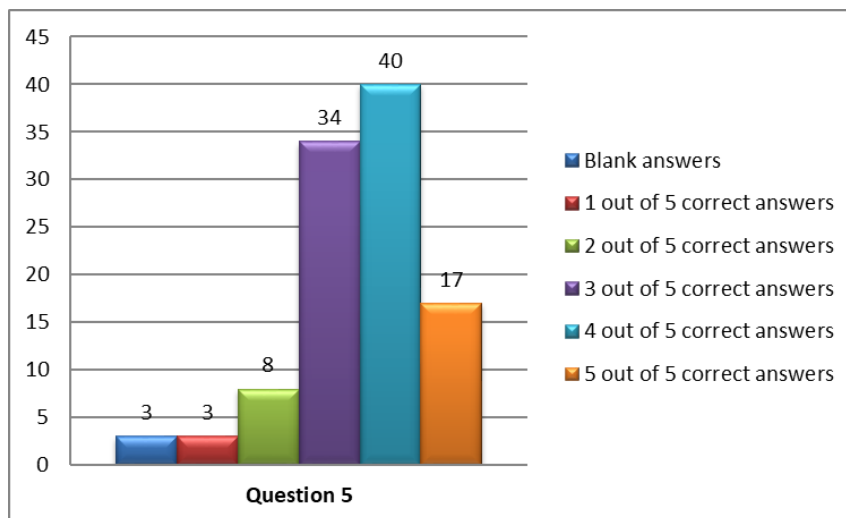


Figure 1.8 Outcomes of the answers to question 5

17 students (16.2%) out of 105 assigned correctly all the T/F, proving able to apply the atomic shell model even to the real cases of neon lamps and fireworks. 40 out of 105 students (38.1%) provided 4 right answers out of 5. Among these, 22 students failed the fifth question, proving unable to recognize the similarities between two real contexts and to transfer their skills from one to another. Overall, this group of students demonstrates some understanding of the theoretical model, without being able to convert this understanding into a skill. The same does not seem true for 34 students (32.4%) who provided 3 right answers out of 5. In fact, these five statements share similar contents, but differ in the form in which information is stated: a correct

understanding should result in mutually consistent answers. The remaining 14 students (13.3%) answered either 1-2 questions or none, showing an insufficient knowledge level. Overall, most students (57 out of 105) provided coherent answers: this suggests understanding or at least familiarity with the atomic shell model and its application to a concrete case, drawn from everyday experience.

Question 6: *Particle representation of distilled water and tap water. Understanding the concepts of substance and mixture and their properties. Use of the particle model*

The image on the left depicts a tank filled with distilled water. The image on the right depicts tap water.

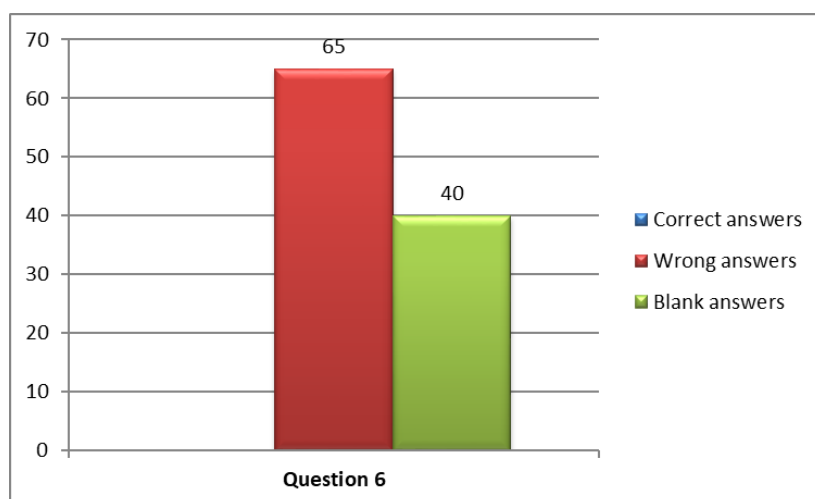


Represents the two systems at the particle level:

Distilled water	Tap water

Complete the following sentences:

1. Tap water boils at a temperature (equal /different) than distilled water.
2. Distilled water contains (one /many) type /s of molecules.
3. Tap water is a (mixture /compound substance).
4. Distilled water is a (mixture /compound substance).



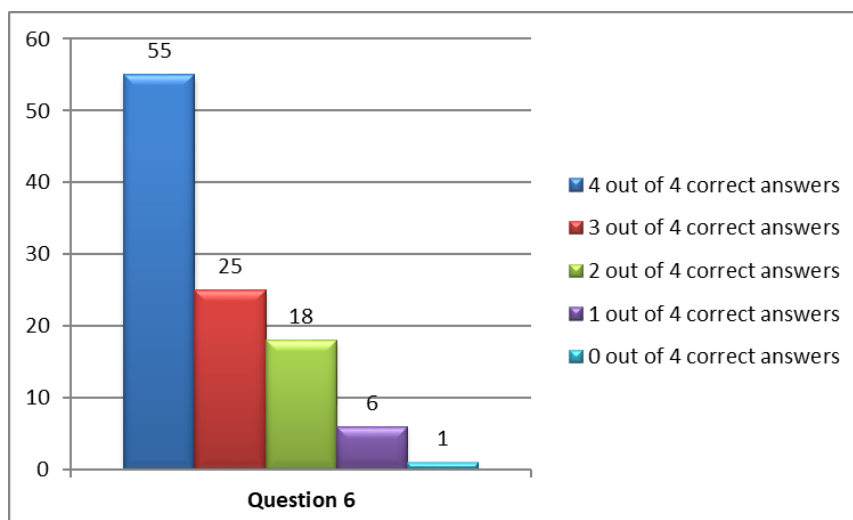
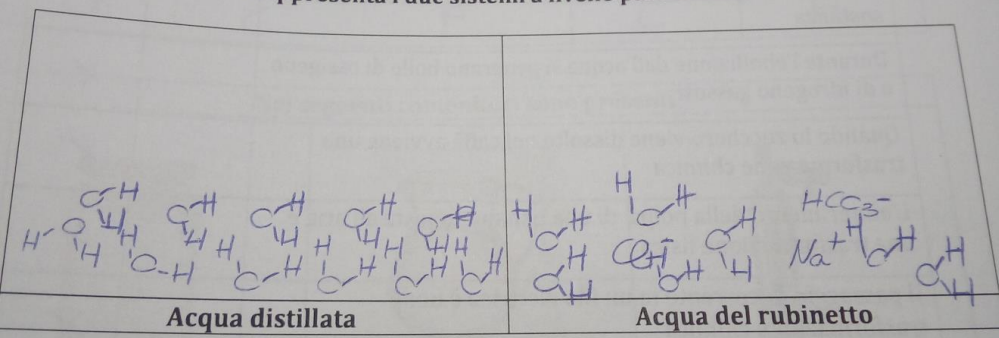
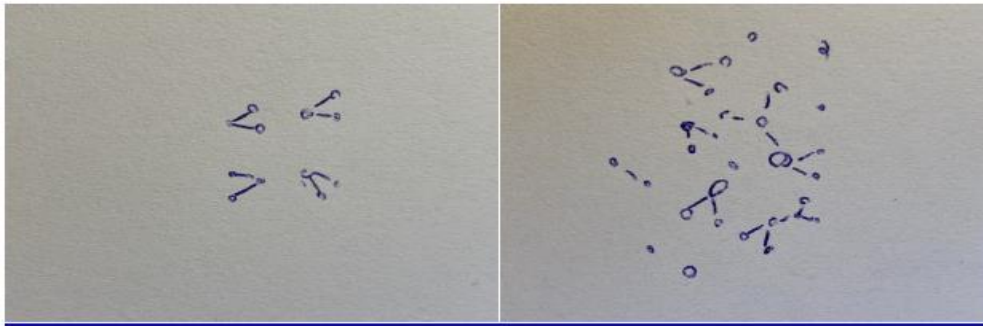


Figure 1.9 Outcomes of the answers to question 6 (particle representations and completion, respectively)

The outcome of this question (as in question 2) highlights the poor understanding and familiarity of students with the particle model of matter and its representations. Only very few representations (figure 1.10) get close to the expected answer (students 8, 62, 64, 100). The expected representations should have taken into account the following aspects: i) liquid state of distilled and tap water in ordinary conditions (particles arranged in a disordered way and close to each other in both boxes); ii) difference between substances and mixtures (single repeated symbol for distilled water and multiple types of repeated symbols for tap water). Students 8 and 64 are the ones who best represent the liquid state, with particles arranged in disorder, but in contact with each other to indicate the condensed state. However, student 8 draws the structural formulas instead of the iconic representations of particles and student 64 represents tap water as a binary mixture (a single chemical species in addition to water). In the other two cases, students represent widely spaced particles, suggesting a gaseous physical state rather than a liquid one.

Student 8	Rappresenta i due sistemi a livello particellare: 
Student 62	

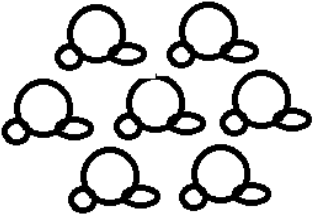
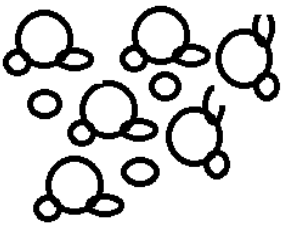
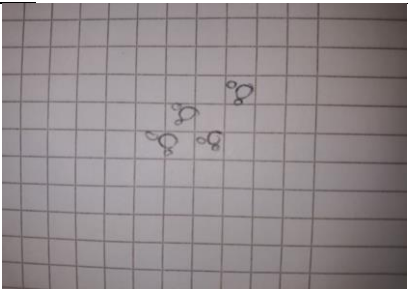
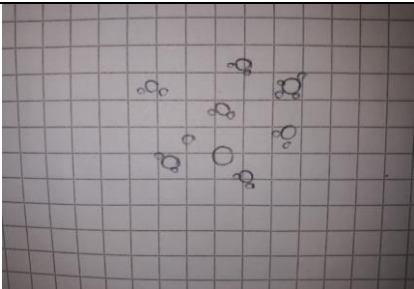
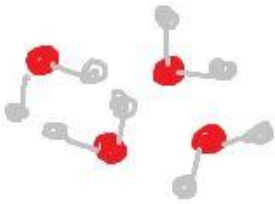
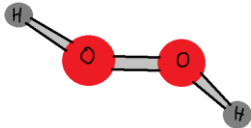
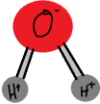
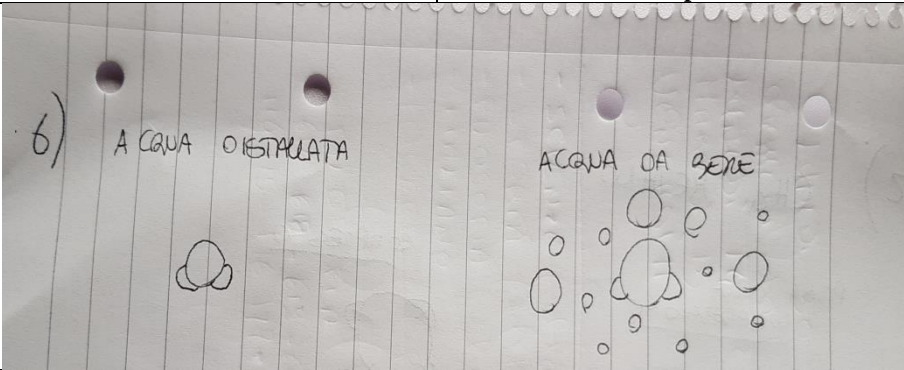
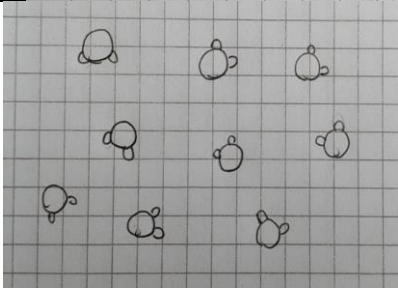
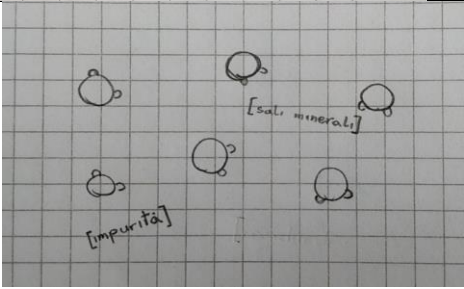
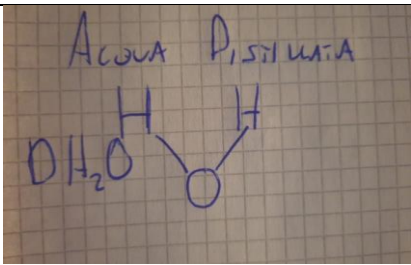
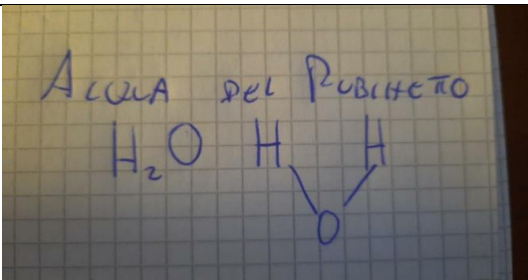
Student 64	DISTILLATA  RUBINETTO 
Student 100	  Distilled water Tap water

Figure 1.10 Particle representations provided by students 8-62-64-100 respectively

Figure 1.11 shows a selection of the most relevant answers. Students 35, 47, 50, 89, 95, 97, 101 recognize tap water as a mixture, but instead of providing the iconic representations, they report brute formulas of water and ions or describe the system in words. Students 88 and 95 replace particle representations with structural and brute formulas and add letter D (probably to mean ‘distilled’) to the brute formula of water. Students 77, 88, and 95 do not recognize the difference between substance and mixture, providing equal symbolic and verbal descriptions in both cases.

Student 35	H ₂ O-SALI (H ₂ O – salts) Distilled water	H ₂ O + SALI (H ₂ O – salts) Tap water
Student 47	 Distilled water	OLTRE ALL' H₂O CI SARANNO ANCHE ALTRI ELEMENTI (IN ADDITION TO H₂O THERE WILL BE ALSO OTHER ELEMENTS) Tap water
Student 50	H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O H₂O Distilled water	H₂O H⁺ H₂O H₂O OH- H₂O H₂O H⁺ H₂O H⁺ H₂O H₂O OH- H₂O H₂O OH- H₂O H₂O OH- H₂O Tap water

Student 51	 Distilled water	 Tap water
Student 54	 Distilled water	Tap water
Student 70		
Student 71	 Distilled water	 Tap water
Student 77	$\begin{array}{cc} \text{H} & \text{H} \\ & \text{O} \end{array}$ Distilled water	$\begin{array}{cc} \text{H} & \text{H} \\ & \text{O} \end{array}$ Tap water
Student 88	 Distilled water	 Tap water
Student 89	ci sono solo molecole di h2o sono disposte ordinatamente (there are only molecules of h2o are arranged neatly) Distilled water	tra le molecole di h2o ci sono anche altri elementi sparsi (among the h2o molecules there are also other scattered elements) Tap water

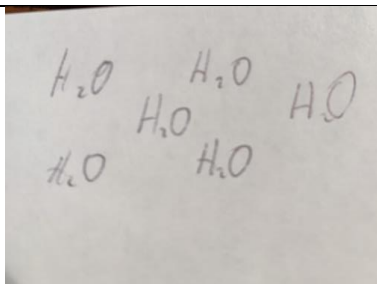
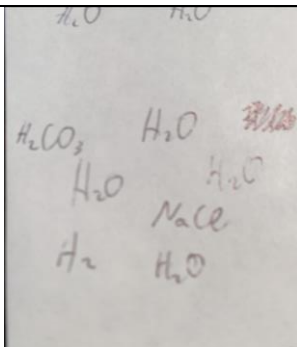
Student 95	DH ₂ O Stessa molecola (Same molecule) Distilled water	H ₂ O Stessa molecola (Same molecule) Tap water
Student 97	Se però l'acqua è distillata, non esistono particelle intorno alle quali le molecole possono addensarsi e ciò rende difficilissimo la condensazione (However if the water is distilled, there are no particles around which the molecules can thicken and makes condensation very difficult)	Particelle chiare in sospensione: sono indice della presenza di calcare. Se l'acqua è ricca di magnesio e calcio, con il calore possono formare piccole particelle bianche, dette "precipitato" (Clear suspended particles: they are an indication of the presence of limestone. If the water is rich in magnesium and calcium, small white particles can form with the heat, called "precipitate")
Student 101	 Distilled water	 Tap water

Figure 1.11 Particle representations provided by students 35-47-50-51-54-70-71-77-88-89-95-97-101 respectively

Student 50 represents distilled water with repeated H₂O formulas, while tap water is described as a mixture of H₂O, OH⁻ and H⁺ ions deriving from the ionic dissociation of the water itself. Clearly he confuses what he learned about the dissociation equilibrium of water with the concept of pure substance and mixture, he also considers ionic species as chemical components distinct from the water substance, whereas no other ionic species are indicated. Student 51 confuses distilled water with hydrogen peroxide: he represents the structural formula of hydrogen peroxide and clearly does not understand the difference between pure substance and mixture. Student 83 makes the same mistake, but reports brute formulas. Both students 70 and 71 report iconic representations, but use them inconsistently. Student 70 represents the water substance as a single molecule: this is a recurring behavior (students 51,54,77,88,95). Furthermore, both students 70 and 71 do not correctly represent the physical state of water, as they draw particles too far apart, rather suggesting the gaseous state. Student 97 reports nonsense sentences in the context of this question. As many as 40 students out of 105 (38%) did not answer, proving unable to represent a pure substance and a mixture (both in the liquid state) at the particle level.

Regarding the second part of the question (sentences to be completed), 55 students (52.4%) complete all sentences correctly (figure 1.9). The correct completions are in the order: different; one; mixture; compound. However, almost all of these 55 students were unable to represent at the particle level what the sentences state, or report inconsistent or incorrect representations (see figure 1.11). 10 out of 13 authors of the representations shown in figure 1.11 (students 35,47,50,51,54,70,71,77, 97 and 101) completed the sentences without making mistakes. Students 88 and 95 only missed the first completion, while student 89 missed completions 3 and 4. This is a symptom of a large gap between the ability to verbally expose theoretical knowledge, its understanding and the ability to provide congruent particle representations of the systems under study. The knowledge seems to have been acquired mostly mnemonically. The students' drawings clearly show how confused, inconsistent and ambiguous their mental models related to the concepts of the microscopic world

are. At the same time, these data denounce the importance of engaging students in particle representations of matter, as they are a very effective tool for detecting student's representations and misrepresentations.

The authors of the representations in figure 1.10 completed all sentences without mistakes: their statements and descriptions were mutually consistent.

All the remaining 50 students missed at least one completion, whereas only student 24 missed all four completions. The set of data indicates a poor and unsatisfactory understanding of the concepts of substance and mixture both at the macroscopic and microscopic levels.

Question 7: *Understanding of the concept of intensive and extensive property and its application to a real context*

You found a coin and need to determine if it is made of pure gold or not.



Which of the following alternatives fit the purpose?

	TRUE	FALSE
I determine its mass		
I determine its density		
I try to break it		
I determine its melting point		
I observe its color		
I use a magnet to check if it attracts the metallic coin		

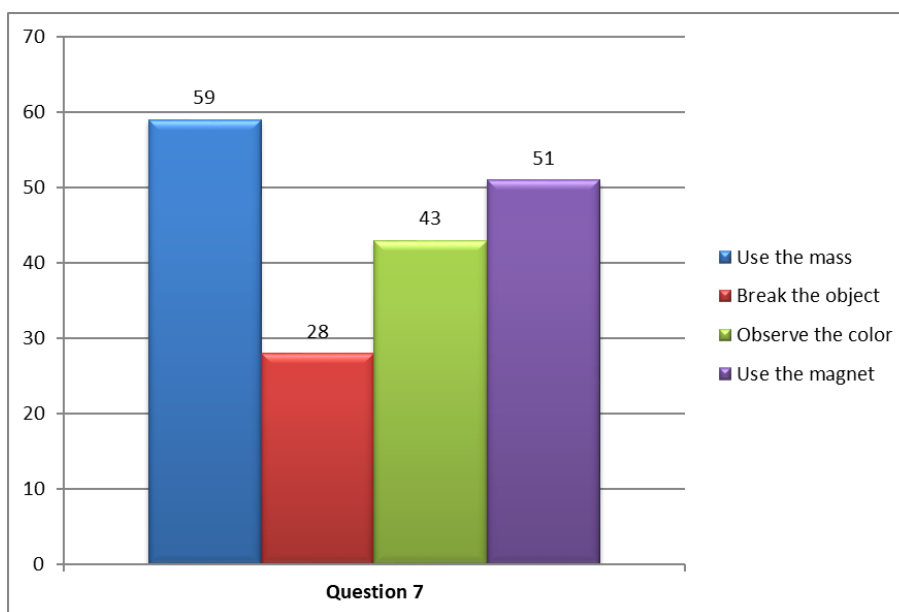


Figure 1.12 Outcomes of the answers to statements 1, 3, 5 and 6 of question 7

Only 5 students out of 105 (<5%) provided a right classification of the 5 statements, proving a good level of understanding of the difference between intensive property (fundamental for the recognition of a substance) and extensive properties. They also proved able to exclude properties of matter, such as color or ferromagnetic properties, which are not suitable for determining whether an object is made of pure gold or not.

The graph in figure 1.12 reports the rate of wrong answers to each question. A relevant percentage of students (56.2%, i.e. 59 students out of 105) seem to believe that a mass measurement can provide information on the chemical composition of an object. Beyond specific skills on extensive and intensive quantities, the use of

logic alone would be sufficient to conclude that the mass cannot provide qualitative information on the objects under examination. Almost half of the sample, exactly 48.6%, believe that the use of the magnet is a suitable option for the recognition of the gold coin, without realizing that the only information obtainable from this test is whether the object contains iron or not. 43 out of 105 students (41%) believe that color is a valid means for recognizing gold. Although gold is characterized by a recognizable color, it is clear that it is not a sufficient requirement to recognize a material: that same color could belong to a gold alloy or to completely different materials, such as brass, pyrite, etc. Finally, 26.7% of the students' sample believe that breaking the object (mechanical property) is an appropriate action for its chemical recognition. The answers to this question reveal a certain naivety, as well as the presence of alternative conceptions regarding the properties of matter.

Question 8: *Understanding the concepts of physical and chemical transformation*

Specify whether the following statements are true or false:	TRUE	FALSE
In a chemical transformation the substances initially found in the system are conserved, in a physical transformation they are not conserved		
Mass is conserved only in physical transformations		
During a chemical transformation the atoms initially found in the system recombine with each other to form substances that are different from the initial ones		
During evaporation, a substance transforms into another substance		
During the boiling of water, gaseous oxygen and hydrogen bubbles are generated		
When sugar is dissolved in coffee, a chemical transformation takes place		
The blackening of the pulp of bananas exposed to air is a physical transformation		
The flow of electricity in an electric wire is a chemical transformation		

The results are shown in Table 1.4. The red color highlights the number of students who provided wrong answers. Only 1 out of 105 students (student 8) answered correctly to all requests.

Specify whether the following statements are true or false:	TRUE	FALSE
In a chemical transformation the substances initially found in the system are conserved, in a physical transformation they are not conserved	24 (22,9%)	81 (77,1%)
Mass is conserved only in physical transformations	29 (27,6%)	76 (72,4)
During a chemical transformation the atoms initially found in the system recombine with each other to form substances that are different from the initial ones	99 (94,3%)	6 (5,7%)
During evaporation, a substance transforms into another substance	21 (20%)	84 (80%)
During the boiling of water, gaseous oxygen and hydrogen bubbles are generated	76 (72,4%)	29 (27,6%)
When sugar is dissolved in coffee, a chemical transformation takes place	62 (59%)	43 (41%)
The blackening of the pulp of bananas exposed to air is a physical transformation	31 (29,5%)	74 (70,5%)
The flow of electricity in an electric wire is a chemical transformation	33 (31,4%)	72 (68,6%)

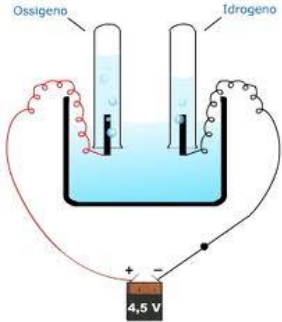
Table 1.4 Outcomes of question 8: in black, the number and% of correct answers; in red, the number and% of wrong answers

The data in the table show that the theoretical understanding of the concepts of chemical and physical transformation and their implications (first four statements) could be improved: in fact, excluding the case of the third question, the other three obtained at least a 20% rate of wrong answers. It is striking that 27.6% of students apply the principle of mass conservation to physical transformations, only. On the other hand, statement 3 is recognized as true by almost all students, including those who do not associate mass conservation with chemical transformations. This suggests that a correct theoretical knowledge does not ensure students' ability to apply it. Probably, students have little practice in using the particle model as a reasoning tool: this might explain their difficulty in associating the conservation of the atoms of various elements with mass conservation.

The outcomes of the application of this knowledge to real situations (last 4 assertions) are much worse than those already discussed. The high percentage (72.4%) of those who associate evaporation of water with formation of gaseous oxygen and hydrogen confirms that this misconception - widely reported by international literature - is widespread (Osborne e Cosgrove 1983; Nakhleh 1992; Mayer 2011). Mayer proposes to use laboratory practice to dismantle it: e.g., the evidence that the product of water evaporation is not explosive suggests that this product cannot be hydrogen. Even the dissolution of polar substances in aqueous environments (e.g. sugar in coffee) is problematic: 59% of students classify it as a chemical process, probably due to the 'disappearance' of the solid substance. The 'disappearance' is often mistaken for an evidence of chemical reactions. Most students seem accustomed to apply their own knowledge/information to new situations mechanically, instead of analyzing it in detail and take into account all possible implications. Once again, the lack of understanding of the dissolution phenomenon might derive from a lack of understanding of the particle model of matter and of the nature of inter-molecular interactions. Had students understood the microscopic model of solvation of polar substances, they would probably recognize dissolution as a physical transformation. Even the application of simple logical correlations is useful: the fact that sugar - with a sweet taste - sweetens the coffee should signal its presence even after dissolution. Had it changed chemically, it would not retain the same properties. These difficulties are recurrent if already Roletto and Mirone (1999) report the difficulties of their students in recognizing the dissolution of sugar as a physical transformation. The authors also report the widespread misconception that a chemical transformation is necessarily an irreversible process. The set of answers to question 8 suggests that many students prefer quick and automatic explanatory schemes (e.g., the solid disappears, so it has chemically changed) to effective explanatory schemes, based on logical and coherent correlations between the analysis of facts and theoretical knowledge. This may be the result of teaching methods that privilege transmissive lessons (which are somehow less demanding) to a didactic path aimed at providing students with effective tools for interpreting reality and metacognitive skills. According to Talanquer (2013), these latter promote rigorous and incisive forms of reasoning.

Question 9: *Understanding of the concepts of physical and chemical transformation. Particle and symbolic representation of electrolysis and evaporation of water.*

After observing the two images below, which refer to substance 'water', provide a representation of the two processes using the particle model and the symbolic language of chemistry.

		
Particle representation		
Symbolic representation		

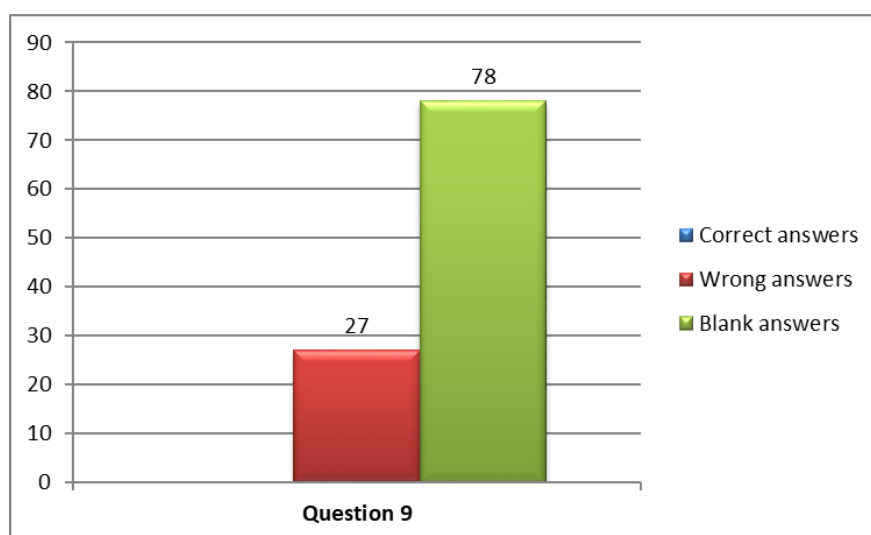


Figure 1.13 Outcomes of the answers relating to question 9

After looking at the images of water electrolysis and evaporation, students are invited to provide the particle and symbolic representations of both. Acceptable representations should take into account: i) liquid state of distilled water in ordinary conditions (particles arranged in a disordered way and close to each other in both boxes); ii) formation of two new substances H_2 and O_2 in the gaseous state, with a consistent iconic representation (water electrolysis); iii) preservation of the identity of the substance represented in the gaseous state, with a consistent iconic representation (water evaporation); iii) conservation of mass (same number of particles in both boxes). The outcome of this question confirms problems in understanding and using the particle model and its iconic representations: as many as 78 out of 105 students (74.3%) did not answer; others provided partial answers, which were often incorrect, or even illogical. Figure 1.14 shows the answers of students 71, 77 and 88. Student 71 confuses macro and micro levels and represents them together. He understands that electrolysis implies a flow of electrons but cannot connect it to the corresponding chemical reaction. Student 77 implies symbolic instead of iconic language; where symbolic representations are requested, he provides verbal descriptions. This may derive from a lack of understanding of these two communicative registers; in addition, he gives the impression to report what he remembers about electrolysis rather than what he has understood. Student 88 reports the structure and the brute formula of water, but is unable to express himself either on the evaporation process or on that of electrolysis.

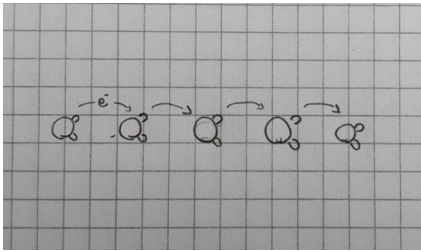
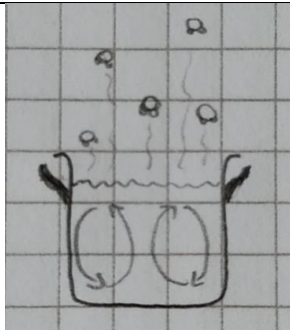
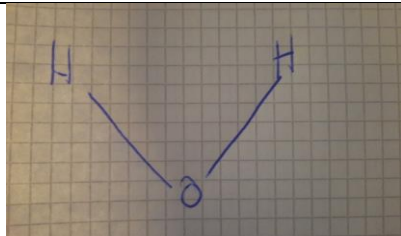
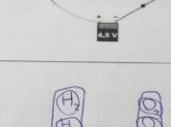
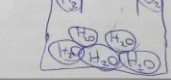
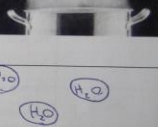
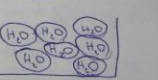
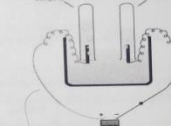
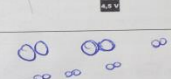
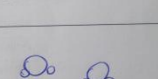
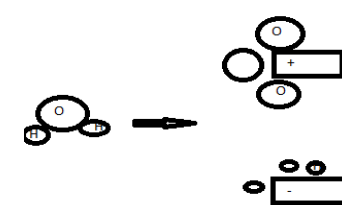
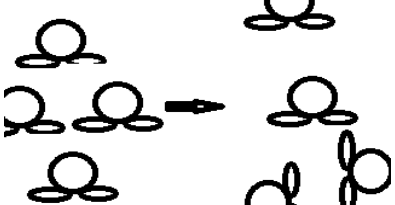
Student 71	Particle representation		
	Symbolic representation		
Student 77	Particle representation	$\text{H}_2\text{O} \rightarrow \text{H}_2 + \text{O}_2$	$\text{H}_2 \quad \text{O}_2$
	Symbolic representation	ELETTROLISI ELETTRODI LEGATI AD ANODO E CATODO ENERGIA ELETTRICA TRASFORMATA IN CHIMICA (ELECTROLYSIS ELECTRODES TIED TO ANODE AND CATHODE ELECTRICITY TRANSFORMED INTO CHEMISTRY)	EVAPORAZIONE DALLO STATO LIQUIDO A GASSOSO (EVAPORATION FROM LIQUID TO GASEOUS STATE)
Student 88	Particle representation		
	Symbolic representation		H_2O

Figure 1.14 Particle and symbolic representations of the electrolysis and water evaporation process of students 71, 77 and 88

Only 8 out of 105 students (7.6%) provided consistent answers to this question, showing a fair level of understanding of the phenomenon (Figure 1.15 reports the answer by students 3, 7, 64, 75, 95 and 101). Nevertheless, two recurring problems are the confusion between iconic and symbolic language and between macroscopic and microscopic levels.

Student 3		 Rappresentazione particellare  Rappresentazione simbolica $\text{H}_2\text{O}_{(l)} + \text{me}^- \rightarrow \text{H}_{2(g)} + \text{O}_{2(g)}$	 Rappresentazione particellare  Rappresentazione simbolica $\text{H}_2\text{O}_{(l)} \rightarrow \text{H}_2\text{O}_{(g)}$
Student 7		 Rappresentazione particellare  Rappresentazione simbolica $2\text{H}_2\text{O} \rightarrow 2\text{H}_2 + \text{O}_2$	 Rappresentazione particellare  Rappresentazione simbolica $\text{H}_2\text{O} \uparrow$
Student 64	Particle representation		
	Symbolic representation	$\text{H}_2\text{O} - \text{electric current} \rightarrow \text{O} + \text{H}$	$\text{H}_2\text{O}(l) -- \text{Heat} \rightarrow \text{H}_2\text{O}(g)$
Student 75	Particle representation	O2 H2 O2 H2 O2 H2 H2O H2O H2O H2O H2O	H2O H2O H2O H2O H2O H2O H2O H2O H2O H2O H2O
	Symbolic representation	$\text{H}_2\text{O} \rightarrow \text{H}_2 + \text{O}_2$	$\text{H}_2\text{O}(\text{LIQUID}) + \text{HEAT} \rightarrow \text{H}_2\text{O}(\text{GASEOUS})$

Student 95			
Student 101	Particle representation		
	Symbolic representation	$\text{H}_2\text{O}(\text{l}) + \text{ELECTRIC CURRENT} \rightarrow \text{O}_2(\text{g}) + \text{H}_2(\text{g})$	$\text{H}_2\text{O}(\text{l}) + \text{HEAT} \rightarrow \text{H}_2\text{O}(\text{g})$

Figure 1.15 Particle and symbolic representations of the process of electrolysis and evaporation of H_2O provided by students 3,7,64,75,95,101

Student 7 provides the best representation as he pays attention to both the quantitative and qualitative aspects of the iconic representation: the number of O and H atoms is unchanged before and after electrolysis, the different substances are clearly represented). Conversely, in water evaporation the liquid state is not consistently represented: only the vapor phase is taken into consideration. However, the persistence of substances in physical transformation is clearly understood and the symbolic and particle representations of the system are consistent with this principle.

Representations of student 95 are interesting in that iconic language is properly used. The qualitative aspects (type of substance and/or elements) of the system are consistent with the particle model, the quantitative aspects are less accurate (no attention is paid to the number of particles). On the other hand, the particle representation of dioxygen and dihydrogen formed by electrolytic splitting of water is incorrect. This student represents individual atoms, instead of diatomic molecules. There is therefore a logical contradiction between this representation and the symbolic one, which instead is correct. In addition, he uses symbols (inverted

commas) whose meaning is not clear. It is interesting to note that all the symbolic representations of Figure 1.15 are correct: the use of symbolic language does not seem problematic. Conversely, most students do not manage iconic language: in fact, they often replace iconic representations with symbolic ones. Student 64 mixes the two types of representations while describing electrolysis. Just like student 95, he draws monoatomic oxygen and hydrogen particles. However, student 64's answers are consistent. Student 3 mixes iconic representations and chemical formulas, as well as macroscopic and microscopic levels. He does not pay attention to the quantitative aspects of the two processes. Student 75 uses the symbolic language only: he tries to represent physical states through a different level of order of the chemical symbols. Similar problems are found in the representations provided by student 101 and in addition, like student 3, student 101 superimposes macroscopic and microscopic aspects. All in all, our conclusions are similar to those expressed for questions 2 and 6.

Question 10: *Understanding of the concepts of physical and chemical transformation and their application to real contexts*

Establish which transformations represented in the boxes below are physical and which are chemical

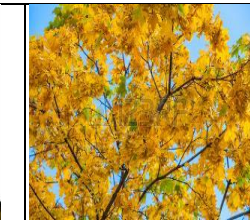
Examples										
	rusty nails		cooking eggs		uncorking a bottle		leaves yellowing		casting of an alloy	
N° answers	92	13	49	56	81	24	83	22	77	28
%	87,6%	12,4%	46,7%	53,3%	77,1%	22,9%	79%	21%	73,3%	26,7%

Table 1.5 Outcomes of question 10. In black: correct answers; in red: wrong answers, and relative percentages

Students were asked to apply their knowledge about chemical and physical transformation, by classifying the processes represented in the pictures. Only 32 out of 105 students (30.5%) provided fully correct answers. Overall, the outcome of question 10 confirm those of the previous two questions: most student have not achieved a meaningful comprehension of the notions of chemical and physical transformation. Data from table 1.5 highlight that egg cooking is the most problematic question: 53% of students class it as a physical transformation, suggesting that cooking implies physical state changes of some substances (e.g. egg white shifts from liquid to solid state). The fact that many foods become edible through the cooking process should prompt students to think that the cooking process involves substance changes: we cannot exclude that, in the absence of a leading criterion, many students answered randomly. Similar considerations can be applied to 26.7% of wrong answers attributed to the casting of an alloy. This result is surprising, as this example is often used in textbooks. The caption might have misled students: “solidification of a metal casting” would have probably generated a lower rate of wrong answers. Unexpectedly, the change of state associated with uncorking a bottle of sparkling wine was recognized by most students, despite the fact that this example is unusual and rather complex. In fact, it requires understanding that carbon dioxide initially dissolved in water is released by virtue of the pressure change. The phenomenon of leaves yellowing misled more than 20% of the students’s sample, who not interpret the macroscopic evidence of a new color as the result of chemical changes occurred in leaves. The most familiar process, namely rust formation, was recognized by a very large percentage of students, probably because it is often mentioned as an example of redox process. Various

scholars (Cokelez et al. 2008; Silva et al. 2016) underline that the distinction between chemical and physical transformation is more complex than the teacher might think, especially if the explanation involves the microscopic level. In this case the student is required to have a good competence of the concepts of atom, molecule, substance, in addition to understanding the distinction between intra- and inter-molecular bonds. Furthermore, the student should know how to link macroscopic evidence to models belonging to the microscopic level. In many cases, this is an obstacle:

“Many students confuse the processes that involve chemical transformations with changes in the physical state backed by their senses, without making use of the scientific models studied in chemistry classes” (Silva et al. 2016).

Question 11: *Understanding of the concept of mole and its application in real contexts*

In the following containers are present		
		
1 Kg of $C_{12}H_{22}O_{11}$	1 Kg of H_2O	1 Kg of O_2
	YES	NO
Do the 3 containers contain the same amount of substance (expressed in moles)?		
Do the 3 containers contain a different number of molecules of each substance?		
In the following containers are present		
		
5 moles of $C_{12}H_{22}O_{11}$	5 moles of H_2O	5 moles of O_2
	YES	NO
Do the 3 containers contain the same mass (expressed in g)?		
Do the 3 containers contain a different number of molecules of each substance?		

Table 1.6 reports the results of question 11. Only 29 out of 105 students (27.6%) provided fully correct answers, and proved able to apply the concept of mole to real contexts. All the others make at least one mistake (33 students), which indicates of an unsatisfactory understanding of the concept.

	YES	NO
Do the 3 containers contain the same amount of substance (expressed in moles)?	14 (13,3%)	91 (86,7%)
Do the 3 containers contain a different number of molecules of each substance?	93 (88,6%)	12 (11,4%)
Do the 3 containers contain the same mass (expressed in g)?	17 (16,2%)	88 (83,8%)
Do the 3 containers contain a different number of molecules of each substance?	62 (59%)	43 (41%)

Table 1.6 Outcomes of question 11. In black: correct answers; in red: wrong answers, and relative percentages

The error rates differentiate the first two questions from the last two to a meaningful extent. The second and fourth questions have the same wording: the former requires a mass-quantity conversion, the latter does not. We would therefore expect a higher rate of right answers in the latter case, which is apparently easier. The outcome of the fourth question suggests that a considerable percentage of students have not understood the meaning and implications of the concept of mole, which allows to handle measurable masses while thinking in terms of particles' number. Wording might have played a role: had we asked "Do the 3 containers contain an equal number of molecules of each substance?", the outcome might have been better. However, the concept of mole is reported to be an obstacle for many students, by virtue of its being a bridge-concept between microscopic and macroscopic levels (particles vs. masses): more than 60 articles related to the mole were published in the last four decades in the Journal of Chemical Education (Fang et al. 2014). As for the Italian context it is worth mentioning an investigation on the understanding of the concept of mole made by Roletto et al. (2003). These authors administered a test to 114 fourth-grade students of two distinct scientific high schools and to 63 students of the third, fourth and fifth grades of the industrial chemistry course of two technical institutes. The results of the study highlighted the inadequate understanding of the definition of mole and of the numerical relationship between atomic or molecular mass and molar mass, in addition to the inability to use the concept of mole operationally, to solve problems.

According to these authors, a possible way out is to exploit analogies between macroscopic and microscopic realms, to solve the problem of quantifying objects that are too small to be directly counted (atoms and molecules): students may be asked to count macroscopic objects by weighting them (e.g. to prepare piles with an equal number of nails, through relative weighting); this allows building up the notion of relative weight; in the third step this notion is applied to microscopic objects. (Roletto et al. 2003).

Question 12: Understanding symbolic language and the meaning of subscripts in brute formulas

The formula of ethyl alcohol is: **C₂H₅OH**

How many H atoms are contained in a single alcohol molecule?	
How many C atoms are contained in a single alcohol molecule?	
How many O atoms are contained in a single alcohol molecule?	

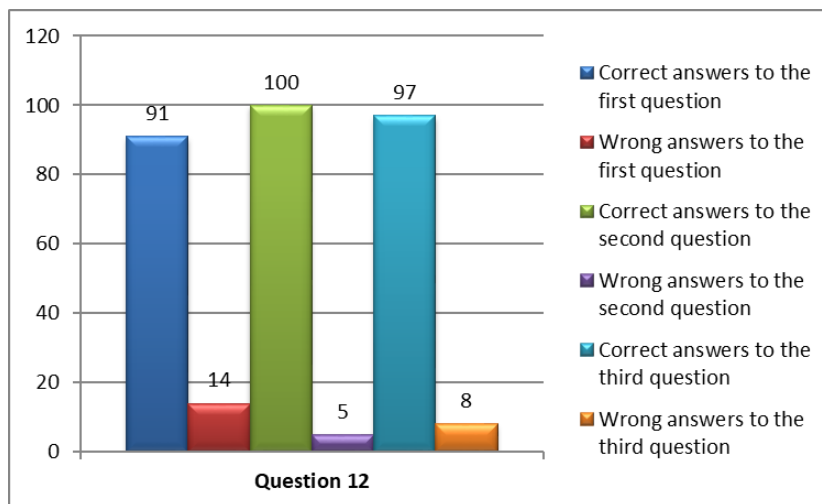
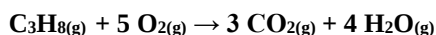


Figure 1.16 Outcomes of question 12

This question posed no significant problems. The expected answers are, respectively: 6; 2; 1. 90 out of 105 students (85.7%) provided correct answers to all these three questions, proving able to interpret the symbolic language of formulas and the meaning of subscripts in brute formulas.

Question 13: Understanding symbolic language and stoichiometric relationships in a chemical equation. Understanding of the concept of quantity of substance.

The combustion of propane is a chemical transformation that can be represented in this way:



- How many CO₂ molecules are obtained by burning 10 propane molecules?
- How many moles of O₂ can react with 4 moles of propane?

	YES	NO
In the laboratory you are asked to weigh 1 molecule of H₂O . Is it possible?		
In the laboratory you are asked to weigh 1 mole of H₂O . Is it possible?		

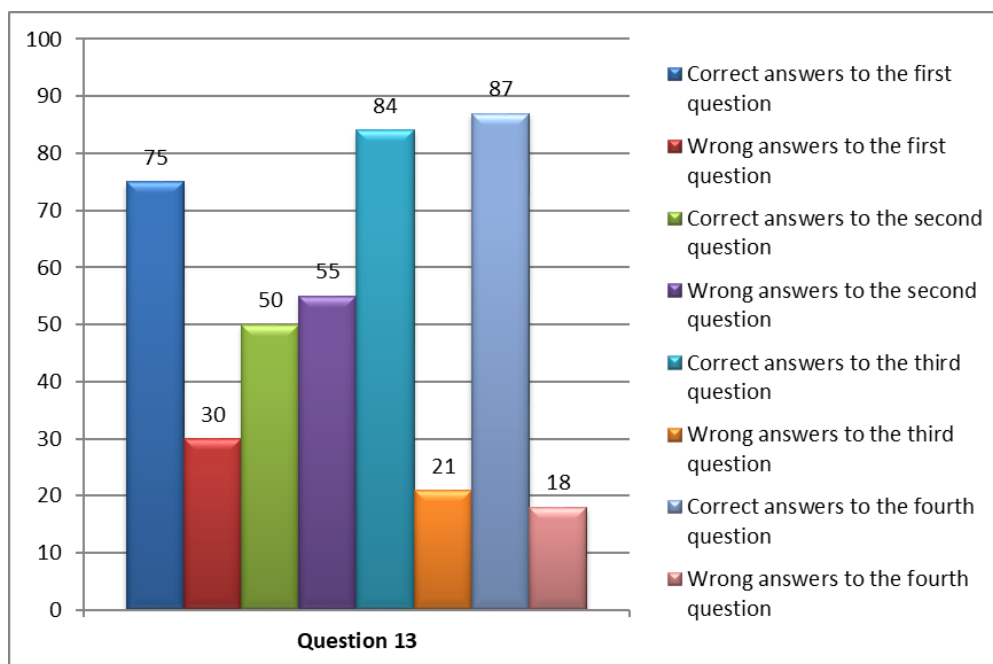


Figure 1.17 Outcomes of question 13

41 out of 105 students (39%) provided all four questions with the expected answers (respectively: 30; 20; NO; YES), proving able to use the notion of ‘quantity of substance’ and to exploit stoichiometric coefficients to calculate reactants and products quantities. More in details, 46 out of 105 students (43.8%) succeeded in answering the first two questions on stoichiometric calculations (the error rate was considerably lower in the first, 28.6%, as compared to the second, 52.4%). Conversely, 76 out of 105 students (72.4%) succeeded in answering the last two questions (which had very similar error rates, 20% and 17.1%, respectively). 71.4% were able to determine the number of CO₂ molecules formed in combustion, whereas only 47.6% of the students’s sample were able to calculate the exact quantity of oxygen consumed by 4 moles of propane. The difficulty is not related to the kind of mathematical calculation (proportion), since both questions require it. The main difference between the two questions concerns the reference to moles rather than molecules. The difficulties encountered by students seem to suggest an unclear understanding of the use of the mole as an index of the number of particles in a system: this is the same problem already highlighted with question 11. Overall, the outcome of this question indicates an unsatisfactory understanding of the concept of mole and stoichiometric ratios.

Question 14: Ability to classify the different types of chemical processes

Assign the reactions represented in the left column (indicated in the right column) to the correct category: indicate the number-letter combination in the central column.

$\text{HNO}_{3(\text{aq})} + \text{KOH}_{(\text{aq})} \longrightarrow \text{KNO}_{3(\text{aq})} + \text{H}_2\text{O}_{(\text{l})}$	1	A Acid-base
$2\text{NaHCO}_{3(\text{s})} \longrightarrow \text{Na}_2\text{CO}_{3(\text{s})} + \text{CO}_{2(\text{g})} + \text{H}_2\text{O}_{(\text{l})}$	2	B Redox
$\text{AgBr}_{(\text{s})} \xrightleftharpoons{\text{acqua}} \text{Ag}^+_{(\text{aq})} + \text{Br}^-_{(\text{aq})}$	3	C Decomposition reaction
$\text{Zn}_{(\text{s})} + 2\text{HCl}_{(\text{aq})} \longrightarrow \text{ZnCl}_{2(\text{aq})} + \text{H}_{2(\text{g})}$	4	D Solubility equilibrium

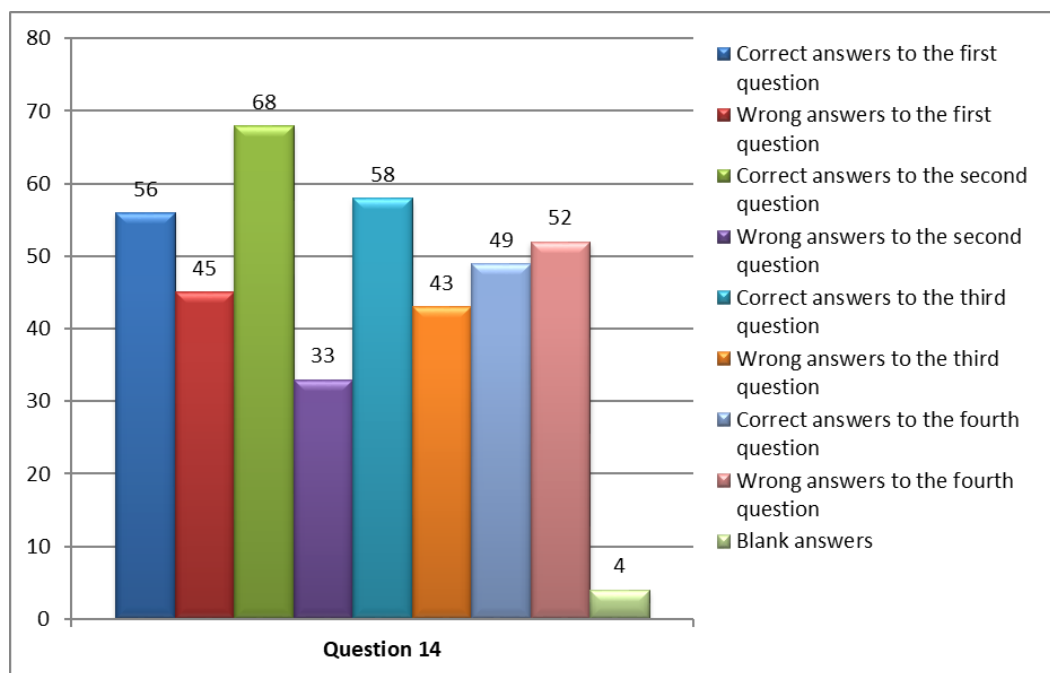


Figure 1.18 Outcomes of question 14

This question asked to assign the correct class to each process. The expected assignments are, respectively: 1-A; 2-C; 3-D; 4-B. Only 32 out of 105 students (30.5%) provided correct classifications of all 4 processes. 40 students (38.1%) made 2 mistakes, 18 students (17.1%) made 3 mistakes, and 10 students (9.5%) failed all associations; 4 students (3.8%) gave blank answers. The processes listed in the table belong to classes of chemical changes that are discussed in any secondary school chemistry course. Acid-base equilibria and redox processes are treated both at the theoretical (modelling) and practical (laboratory) levels; in addition, they are also discussed in disciplinary fields other than chemistry (e.g. biology). As a consequence, all students have certainly been exposed to the didactic treatment of these reaction models during their career: the lack of recognition of the various reaction types suggests that they have been the object of mnemonic learning, without becoming part of the students' cognitive heritage.

Question 15: Understanding bonding models

Complete the following sentences:

1. The dihydrogen molecule is formed when two individual hydrogen atoms bond together. This happens because the dihydrogen molecule is (more / less) stable as compared to the two isolated atoms.
2. The (covalent / metallic) bond that links the two hydrogen atoms in the dihydrogen molecule implies sharing a pair of (protons / electrons).
3. The methane hydrocarbon molecules behave like..... (instantaneous / permanent) dipoles.
4. In the HCl molecule an electric dipole..... (is / is not) found: in this molecule the barycentres of positive and negative charges (coincide / do not coincide).
5. If polar bonds are present in a molecule, the molecule (will / will not be) certainly polar.
6. A molecule that contains only (polar / apolar) bonds is certainly apolar.
7. Substance H_2O at room temperature is in the liquid state whereas substance H_2S is in the gaseous state: in the first case, intermolecular chemical bonds are (stronger / weaker) as compared to the second.
8. In substance NaCl the (covalent / ionic) bond is due to the electrostatic attraction between (molecules / ions).
9. Common sugar is soluble in water because its molecules are (polar / apolar).

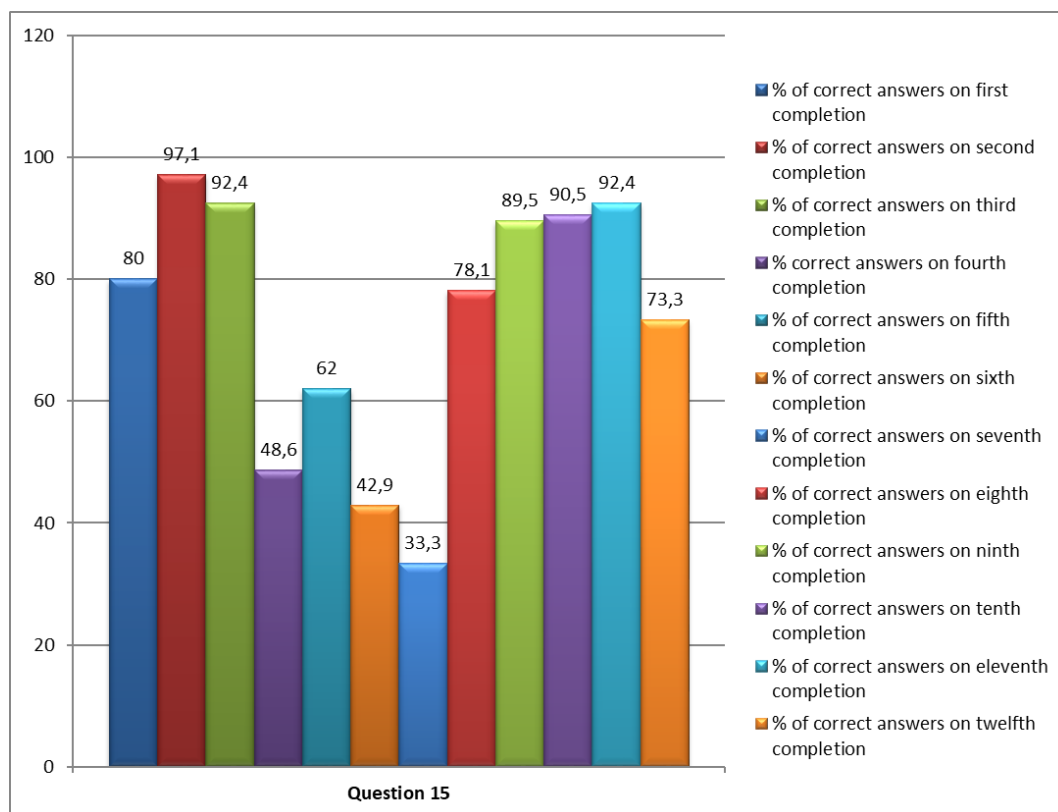


Figure 19. Outcomes of question 15

This question asked to complete nine sentences focused on the concepts of intra- and inter-molecular interactions, polarity of molecules, instant and permanent dipoles, by choosing between two possible alternatives. The expected choices are, respectively: 1) more; 2) covalent and electrons; 3) instantaneous; 4) is and do not coincide; 5) will not be; 6) apolar; 7) stronger; 8) ionic and ions; 9) polar. The aim was to ascertain the level of knowledge of chemical bonding models, and the relationship between bond polarity and molecule polarity. Only 3 out of 105 students (2.9%) completed all sentences (12 completions) without any mistake. 11 students (10.5%) made only 1 mistake, 25 students (23.8%) made 2 mistakes, 20 students (19%) made 3 mistakes, 19 students (18.1%) made 4 mistakes, 16 students (15.2%) made 5 errors, 7 students (6.7 %) made 6 errors, 2 students (1.9%) made 7 errors. Only 1 student made 9 errors and another one did not answer (1.9%). 21 students were not able to relate the formation of the dihydrogen molecule with energetic reasons. Energy issues inherent bonds formation are often overlooked, although they might be easily discussed using the Lennard-Jones graph (Bergqvist et al. 2016).

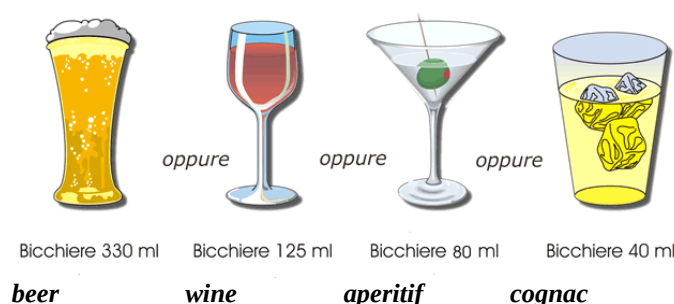
Only 3 students mistook covalent and metallic bonds, probably because the considerable differences in the properties of metallic and covalent substances are well known to the students. Quite unexpectedly, 8 students (7.6%) identified protons as part of the bonding pair. The error, even if limited to a small percentage, is quite serious because it denounces the lack of understanding of the role of electrons in the chemical bond and, possibly, of the Lewis model. 54 students (over 50% of the sample) were not able to associate the presence of instantaneous dipoles with methane molecules, while 40 students (38%) did not recognize the molecule of hydrochloric acid as a permanent dipole. The relationship between charge distribution and presence/absence of dipoles was problematic for a large part of the sample (60 students, 57.1%, missed the second completion of the fourth sentence). Here we detect the students' difficulty in elaborating the concept of (instantaneous and permanent) dipole, that is widely denounced in the literature (Ünal et al. 2006; Coll and Taylor 2001; Peterson and Treagust 1989). An effective understanding of the concept of dipole implies awareness of the mobility of electrons and its implications (symmetry or asymmetry of charge distribution, coincidence or non-coincidence of the centers of gravity of positive and negative charges within a molecule). Unfortunately, the consequences

of electron mobility are poorly discussed in the school context. Not for nothing, several studies denounce the spread of many alternative conceptions on these concepts (Ünal et al. 2006; Coll and Taylor 2001; Peterson and Treagust 1989). A further conceptual difficulty lies in the connection between polarity and molecular geometry: this is confirmed by the outcome of sentence 5, which sees 70 wrong answers out of 105 (66.7%). Sentence 6, concerning the same topic, has better results than the previous one (only 23 pupils out of 105, 21.9%, provided unacceptable answers) and takes into consideration the case of a non-polar molecule. Taken together, the results of sentences 5 and 6 suggest that students reason according to an automatism that leads them to associate polarity/apolarity of bonds with polarity/apolarity of the corresponding molecules, without taking into account molecular geometry. Completion of sentence 7 did not raise significant problems (94 out of 105 students, or 89.5%, answered correctly): the students were able to correlate the magnitude of intermolecular forces with the physical state of the two substances. Sentence 8 also seems to raise no problem (the two sentences were completed correctly by 90.5% and 92.4% of the students's population, respectively). The choice of a substance that is familiar to students and widely cited by textbooks as paradigmatic example of ionic compounds probably concurred to this positive outcome. Literature data show that the misconception according to which ionic compounds are made up of molecules is widespread (Taber 1997).

Finally, completion of sentence 9 raised problems for 28 out of 105 students (26.7%), which classify sugar as non-polar substance. This sentence implies the correct understanding of the concept of molecular polarity and knowledge of intermolecular interactions. This outcome taken together with the results of sentences 5, 6 and 7 suggests that a significant percentage of students did not understand these concepts and/or do not know how to apply them in a real context. Question 15 touches on several issues related to the concept of bonding, which is a foundational chemical notion, relevant to many other disciplines (e.g. biology and biochemistry). Overall, the outcome was satisfactory: 59 out of 105 students (56.2%) made a maximum of 3 errors out of 12 completions; 78 out of 105 students (26.7%) made a maximum of 4 errors. However, the analysis of the answers based on the concepts of temporary and permanent dipoles and molecule polarity highlight gaps in the understanding of these concepts and in the students' ability to apply their knowledge to real cases. Overall, the data are in line with literature studies, that witness the widespread presence of various misconceptions on aspects of chemical bonding, such as the connection between the type of transformation undergone by a system and the type of interatomic interaction involved in it (Nahum et al. 2010; Schmidt et al. 2009; Cooper et al. 2015) or the energetic aspects involved in the different types of bonds (Coll and Taylor 2001).

Question 16: *Understanding the concept of concentration as an intensive property*

Look at the following picture:



All three glasses contain exactly 12g of alcohol

	beer	wine		aperitif	cognac
In your opinion, which drink is characterised by the highest alcoholic concentration?					
The alcoholic concentration in the aperitif is exactly half the concentration in another drink: which one?					

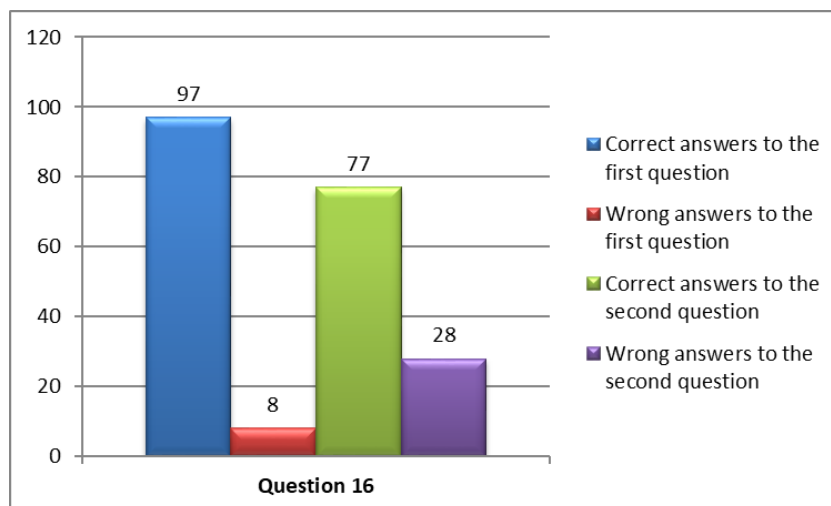


Figure 1.20 Outcomes of question 16

Understanding the concept of concentration and its character of intensive property is a well-known learning obstacle. However, 70.5% of the sample (74 out of 105 students) proved capable of answering both questions correctly (the expected answer for both questions is: cognac). 26 out of 105 students (24.7%) gave only one wrong answer, and only 5 students (4.8%) got both wrong. Conceptually, the second question presents more obstacles than the first. In fact, the first question implies the simple comparison of volumes. The second one implies knowing the concept of intensive property and the inverse proportionality between concentration and volume. The general outcome of question 16 suggests that the majority of students have adequately understood these concepts.

Question 17: *Understanding the concept of intensive quantity, concentration and dilution of a solution.*

The beer contained in this bottle has a 5% v/v alcoholic rate Pour a little into a glass:



Is the alcohol concentration in the beer poured into the glass different from that of the entire bottle?		
Is the amount of alcohol in the beer contained in the glass different from that of the entire bottle?		
Add water to the beer previously poured into the glass. Has the alcohol concentration in beer changed after adding water?		
Has the beer in the previous example been diluted?		
Pour 300 ml of beer (5% V / V) into the glass and add 300 ml of water. The concentration became 10% V / V		

This question involves the application of the concept of concentration, dilution and the comparison between intensive and extensive properties.

53 out of 105 students (50.5%) performed the entire exercise correctly, proving able to use the concepts of concentration and dilution of a solution and to distinguish between intensive and extensive quantities. Table 1.7 shows the detailed analysis of students' answers.

	YES	NO
Is the alcohol concentration in the beer poured into the glass different from that of the entire bottle?	16 (15,2%)	89 (84,8%)
Is the amount of alcohol contained in the glass of beer different from that in the entire bottle?	82 (78,1%)	23 (21,9%)
Add water to the beer previously poured into the glass. Has the alcohol concentration changed after adding water?	92 (87,6%)	13 (12,4%)
Has the beer in the previous example been diluted?	96 (91,4%)	9 (8,6%)
Pour 300 ml of beer (5% v/v alcoholic rate) into the glass and add 300 ml of water. The alcoholic concentration has become 10% v/v	14 (13,3%)	91 (86,7%)

Table 1.7 Outcomes of question 17. In black: correct answers; in red: wrong answers (number of students and%)

The comparison between the first and the second question shows that approximately 20% of the students's sample did not understand the difference between extensive and intensive quantities, as they confuse concentration and quantity of solute found in a given volume of solution. The last three questions are linked and focus on the concept of dilution: 9, 12 and 13% of students's sample, respectively, proved unable to apply this concept correctly. A comparison between the rate of wrong answers concerning the concepts of intensive and extensive property (first two questions) and the rate of wrong answers concerning the notion of dilution (questions 3, 4 and 5) shows no correlations between these two outcomes. Overall, the results indicate a satisfactory level of understanding of the concepts of dilution and concentration.

Question 18: Understanding what is classified in the periodic table of elements.

Which of the following items are present in the periodic table of elements?		
	YES	NO
H ₂ O		
Elementary substance dihydrogen (H ₂)		
Hydrogen element (H)		
Steel		
Artificial elements		
Atomic number		
Quartz		
Only metals		
Atomic mass		
Molar mass		

Which of the following items are present in the periodic table of elements?		
	YES	NO
H ₂ O	8 (7,6%)	97 (92,4%)
Elementary substance dihydrogen (H ₂)	6 (5,7%)	99 (94,3%)
Hydrogen element (H)	103 (98,1%)	2 (1,9%)
Steel	30 (28,6%)	75 (71,4%)
Artificial elements	61 (58,1%)	44 (41,9%)
Atomic number	103 (98,1%)	2 (1,9%)
Quartz	21 (20%)	84 (80%)
Only metals	32 (30,5%)	73 (69,5%)
Atomic mass	100 (95,2%)	5 (4,8%)
Molar mass	72 (68,6%)	33 (31,4%)

Table 1.8 Outcomes of question 18. In black: correct answers; in red: wrong answers (number of students and %)

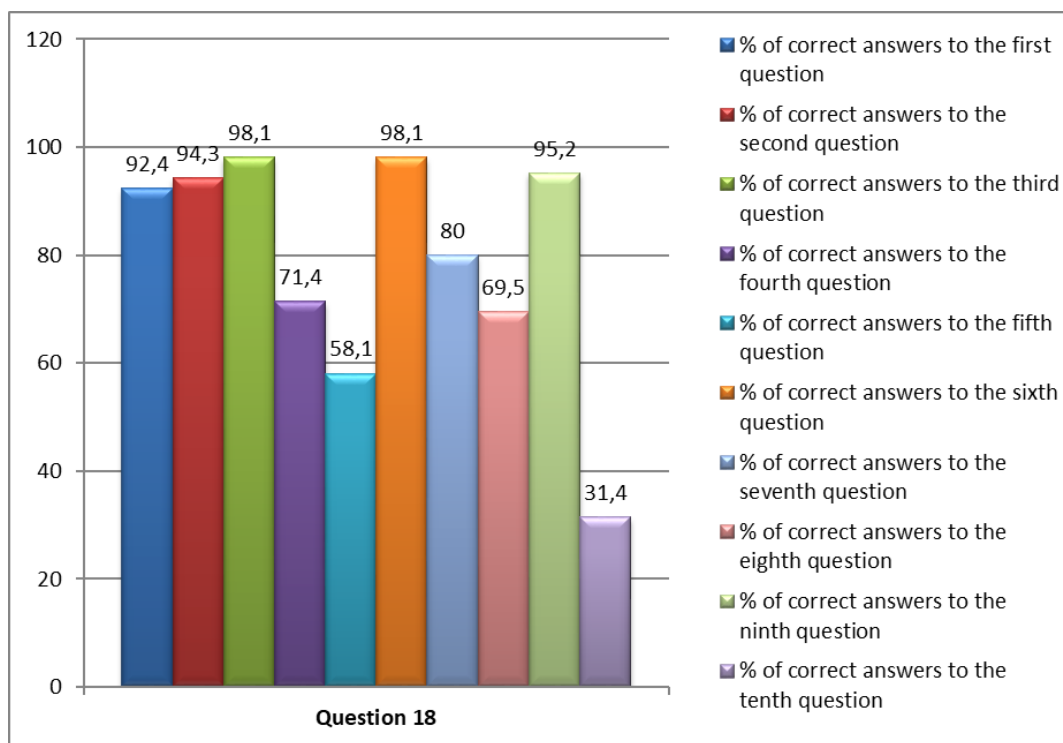


Figure 1.21 Outcomes of the answers relating to question 18

Only 14 out of 105 students (13.3%) correctly identified all items. 22 students (21%) made 1 mistake, 33 students (31.4%) made 2 mistakes, 22 students (21%) made 3 mistakes, 8 students (7.6%) made 4 mistakes and 4 students (3.8 %) make 5 mistakes. 1 student made 7 mistakes and 1 student did not answer. A high percentage of correct answers was collected for all those items that, previously, had been openly discussed in the classroom (element, atomic mass, atomic number) or were related to familiar substances (water). The percentage decreases for items dealing with less familiar substances (quartz). Steel mistook 28.6% of students's sample, who probably take it as a pure metal. The percentage of students who did not contemplate the presence of artificial elements is high (41.9%), probably because these elements are rarely dealt with at school. 30.5% of students's sample seem to believe that the periodic table contains only metallic elements: this question might have been misunderstood, given the emphasis that is usually placed on the distinction between between metals and non-metals when introducing the periodic table. Finally, 68.6% believe that the molar mass is included in the periodic table, a result likely generated by the ambiguous use of the terms atomic mass and molar mass.

1.3. Conclusions

Aim of this survey carried out on a limited sample of students in terminal classes of secondary schools was to verify their basic chemical skills. For this reason, the questions span on a range of basic chemical concepts, sometimes presented in everyday life contexts. The use of different types of question (multiple choice, sentence completion, etc.) was intended to limit the impact of the type of questions on the overall outcome; the application of concepts to real-life situations aimed at verifying students' ability to extend the application of their chemical knowledge to non-schoolish contexts. Our results suggest poor understanding of many basic concepts and lack of ability to think chemically.

The most problematic issues were:

- particle model of matter and its iconic representations (questions 2-4-6-9);
- concept of elementary substance and compound, as well as substance and mixture (questions 4 and 6);

- relationship between quantity of substance and mass (question 11);
- concepts of physical and chemical transformation and their discriminating criteria (questions 6 and 8);
- concepts of instantaneous and permanent dipole / bond polarity / molecule polarity (question 15).

The students' answers highlighted several misconceptions, particularly in questions 7-8-10-15-18.

An acceptable or good degree of understanding of the following topics was also detected:

- interpretation of chemical formulas and meaning of subscripts (question 12);
- correlation between entities of intermolecular forces with the physical state of substances (question 15);
- relationship between ionic bond and electrostatic attraction between charges of opposite sign (question 15);
- notions of concentration and dilution (questions 16 and 17).

In general, whenever students were asked to carry out complex reasoning, or correlations between concepts or applications of theoretical concepts to real situations, a significant percentage of the sample had problems. The emphasis put on interdisciplinary approaches to science learning is challenged by these results: in fact, insufficient understanding of foundational concepts is an obstacle to the understanding of more advanced contents in chemistry courses (e.g. thermochemistry, kinetics, chemical equilibrium, electrochemistry, organic reactivity) and in those of related disciplines (e.g. biochemistry):

“Failure to master basic knowledge can therefore constitute a real impediment to learning advanced concepts; the presence of misconceptions may lead to learning new knowledge in a different way” (Mirone e Roletto 1999).

Despite the local and partial character of this survey, carried out in few schools, with a mere explorative aim, its outcomes confirm the results of previous studies carried out during the last 20 years in Italy (Rihab e Cardellini 2011; Carrozza 2005; Roletto et al. 2003; Mirone e Benedetti 2001). This suggests that the level of chemical understanding amongst Italian high school students has not changed significantly over the years. It has to be borne in mind that similar problems are reported by the international literature in the field.

Overall, these results indicate a problematic situation that originates from various factors: i) the intrinsic difficulty of many chemical concepts; ii) the abstractness of the theoretical interpretations of chemistry, which refer to the atomic-molecular world, inaccessible to perception; iii) the limited effectiveness of teaching practices that privilege mnemonic learning over meaningful learning;

iv) an Italian peculiarity, namely the fact that chemistry is often taught by teachers that have a disciplinary background other than chemistry³; hence they often lack the habit to think chemically⁴.

A good teaching practice of chemistry (and, in general, of science) should:

- insist on the notion of model and its relationship with real systems, as the necessary epistemological premise to any scientific discourse. This implies clarifying the link between the macroscopic level of

³ In Italy there is a teaching qualification class designated as A050 (natural, chemical and biological sciences). This qualification class can be accessed by teachers with quite different disciplinary training (chemists, biologists, geologists, etc.).

⁴ The way of thinking of a chemist is qualified by the consistent use of ideas that pertain to three distinct conceptual levels: macroscopic, microscopic and symbolic. Thinking chemically implies the need to consciously use abstractions that pertain to different conceptual planes. The meaning of the term 'Thinking chemically' is well illustrated by Luigi Cerruti when he observes that chemists perceive "changes in color, the formation of a precipitate, the development of a gas, etc." and, in a way that is all but obvious, they interpret these processes as "the result of events involving invisible particles" (Cerruti 2019).

empirical phenomena and the microscopic level of modelling (Johnstone 2010, Nelson 2002), that fulfils the explanatory needs raised by the phenomenological level;

- rely on a recursive approach to concepts; pay attention to conceptual prerequisites (Roletto 2005);
- clarify the relationship between the three levels of Johnstone's triangle (Johnstone 2010), in order to maximize meaningful learning and avoid fostering misconceptions: "Teachers rarely care emphasizing that these two levels, albeit linked by multiple and very close relationships, are distinct; hence, the need not to confuse them by applying terms and concepts belonging to the macroscopic level to descriptions pertaining the submicroscopic level, or vice versa, which is often the case with the pairs element-atom, substance-molecule, combination-bond, etc. Mixing up the two levels inevitably concur making the comprehension of their relationships more difficult and strengthen the obstacles to chemistry learning even at university level" (Mirone and Roletto, 1999);
- adopt teaching practices that take students as actors, instead of passive subjects, of the learning process. In this perspective, traditional lessons loose ground in favor of activities aimed at developing students' critical sense and logical and social skills (Aimi et al. 2008; Cardellini 2018, 2016; Cardellini and Johnstone 2015; Carrozza and Michelon 2007; Fiorentini et al. 2007; Giuliano 2011; Roletto 2005).
- the investigation of the students' initial conceptions (Mirone and Roletto 1999).

This brief survey highlights the need for a strong renewal of chemistry teaching in schools, aimed at promoting a better understanding of this subject by students.

Relevant benefits of this action are:

- To train informed citizens, capable of critical choices and independent thinking, e.g. people able to discern between well founded information and fake news. According to Lagowski: "We don't need more students who specialize in scientific disciplines; we need to have all other students better informed in science, because they represent the vast majority of future citizens" (Lagowski 1991, cited in Rihab and Cardellini 2011).
- To equip those students who will pursue scientific studies with adequate conceptual bases for understanding the most advanced interpretive models. In fact, Mirone e Roletto (1999) remark that: "The acquisition of basic scientific concepts is essential to understand more advanced concepts. In other words, basic concepts, considered trivial by those who already master a discipline, must be metabolized by students who need to integrate them into their mental schemes in order to use them as foundations for more advanced learning. *Failure to master basic knowledge, considered obvious by university teachers, can therefore represent a significant obstacle to the acquisition of specialized knowledge*" (our translation, italics added).

Disciplinary didactic research can contribute to satisfying this need by promoting good practices of didactic transposition that cannot ignore the following aspects:

- ✓ the theoretical-conceptual aspects of the knowledge to be taught;
- ✓ the didactic strategies and devices used by teachers;
- ✓ the cognitive and pedagogical aspects;
- ✓ the investigation of the students' initial conceptions.

The improvement of the quality of chemistry teaching/learning outcomes in Italy can be promoted by building collaboration nets between academic didactic research groups and science teachers working in Italian secondary schools.

This PhD project is inscribed in this perspective. In fact, the author of this thesis is a tenured chemistry teacher (teaching classes A034 and A050): once trained to didactic chemical research, she will disseminate the results and methods of her research work among her colleagues, encouraging the practice of new and more effective teaching actions.

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Chapter 2

Educational research on the concept of chemical bonding: state of the art and theoretical premises for the development of a didactic sequence

Introduction

This PhD project aims at tackling some educational needs that emerged in the context of the debate over chemical education, appeared in the literature in the last twenty years. The ultimate aim of this PhD thesis is the design of a didactic sequence on intra- and inter-molecular chemical bonding, addressed preferentially to students of the first two years of secondary school. The elaboration of a didactic sequence, i.e. a concrete operational tool to be offered to teachers of upper secondary schools, is a contribute whose meaning lies in the need to bridge the gap between educational didactic research and daily teaching practices.

Paolo Mirone (Mirone 2001) notes that:

“Researchers in didactics, for understandable career considerations, tend to publish the results of their studies in the most established international journals, which, however, are found only in some university libraries and are read almost exclusively by other researchers, being difficult to access to most secondary school teachers.

A further difficulty is represented by the fact that, often, the authors of these publications do not bother to 'translate' the results of their research into indications that can concretely help teachers to modify their teaching practice” (Mirone 2001, my translation).

The fact that the author of the present research project is an experienced chemistry teacher (belonging to the Italian teaching class A034 and A050, i.e. chemistry for technical studies and chemistry in Liceum, respectively), is relevant in view of bringing the academic world of didactic research closer to the school environment.

From this point of view, the present research project is an example of *good practices* whose aim is not the construction of the hybrid figure of 'teacher-researcher'. It rather points at the dissemination of research results in the school environment, thanks to teachers who - after having been trained in the practice of didactic research – go back to school and act as *secondary sources* in the school system, thus promoting innovative teaching practices among their own colleagues.

The choice of working on the issue of chemical bonding (please note that, by this term, we mean all kinds of interatomic interactions) arises from the following reflections:

- ✓ Chemical bonding is a foundational chemical concept, involved in all phenomena related to the reactivity of substances
- ✓ It is essential for justifying the properties of substances
- ✓ It acts as interpretive key at the microscopic level, to explain the behavior of the material realm
- ✓ It is necessary for understanding the contents of other disciplines, such as biochemistry and biology. For example, the DNA double helix is structured by hydrogen bonds; the levels of protein structure depend on the types of inter-atomic interactions involved; at the base of the complexity of the cell membrane there are chemical-physical interactions, etc.

- ✓ It allows facing various didactic problems such as: the use of models, the relationship between macroscopic and microscopic levels, the historical-epistemological evolution of disciplinary concepts and the didactic role that this evolution can play, the use of explanatory schemes and mnemonic devices in teaching-learning processes, the concept of classification and its use, the emergence of alternative conceptions.

The two main purposes of our didactic sequence are motivational and didactic, respectively. On one side, it is important to provide satisfactory answers to the explanatory needs of students, which are spontaneously connected to the macroscopic world, i.e. the experiential world. This implies giving students the opportunity to find plausible answers to questions such as: Why are metals conductive and plastics insulating? Why are salts fragile? Why is diamond so hard? Why is sugar soluble in water whereas oil it is not? Why does ice float on liquid water? Etc... In fact, it is crucial to stimulate students' interest in investigating phenomena with clear practical evidence through a scientific approach. The second purpose is to limit the emergence of alternative conceptions on the notion of chemical bonding or to avoid feeding those already present in students.

Our sequence is grounded on didactic-pedagogical choices that are based on the results of the educational research on the issue of chemical bonding. Hence, this thesis work is inscribed in the frame of the didactic and pedagogical research landscape available on chemical bonding. As a first step, we made a survey of the recent literature by using the following questions as guidelines:

- ✓ Which are the main concepts related to the topic of intra- and inter-molecular chemical bonds that must be the object of didactic transposition?
- ✓ Which are the methodological aspects and didactic strategies commonly adopted in teaching these topics?
- ✓ Which didactic approaches and strategies foster a meaningful learning of intra- and inter-molecular chemical bonds?
- ✓ Which are the most common alternative conceptions regarding these issues and where they come from?
- ✓ Which teaching approaches and strategies hinder the emergence of alternative conceptions regarding intra- and inter-molecular chemical bonds?

2.1 Some methodological notes

The bibliographic searches were carried out using the following databases: Web of Science, Scopus, Scifinder and directly on the website of the main international journals such as the Journal of Chemical Education (American Chemical Society), Chemistry Education Research and Practice (Royal Society of Chemistry) and Recherches en didactique des sciences et des technologies (RDST, École Normale Supérieure, Francia). We used the following keywords:

- chemical bond and chemical education in secondary school;
- chemical bonding concept and secondary school;
- chemical bonding approach and secondary school;
- chemical bond alternative conception and secondary school;
- teaching approach chemical bond and secondary school.

We mainly focused on the time interval from 1995 to 2018, and we went back to other relevant sources through the bibliography of the articles that had been selected at the beginning.

Following the principles of the Sistematic Review (Saiani and Brugnolli 2010), the information was managed through the compilation of summary tables, or data-extraction tables, structured in 5 columns (bibliographic reference, title of the article, learning context, methodological approach, summary of results and conclusions) according to the following example:

BIBLIOGRAPHIC REFERENCE	TITLE	CONTEXT	METHODOLOGICAL APPROACH	SUMMARY AND CONCLUSIONS
Jarkko Joki, Jari Lavonen, Kalle Juutib and Maija Akselaa Chem.Educ.Res.Pract., 2015, 16,901-917	Coulombic interaction in Finnish middle school chemistry: a systemic perspective on students' conceptual structure of chemical bonding	The new method for teaching chemical bonding was applied in a Finnish school along three years (7th grade to 9th grade); it involved 38 students divided into three groups. The school is located in southern Finland in an urban area and the students come mainly from the middle and upper social classes.	The purpose of this research is to emphasize the use of Coulomb interactions as a foundation for learning all types of chemical bonds. Another aim is to investigate the conceptual structures of middle school students concerning the chemical bond, through a systemic perspective, which attempts to synthesize the different levels at which conceptual structures can be considered.	The most significant problem for teaching chemical bonding is not the octet rule, but rather the balance between the use of explanatory schemes and mnemonic devices. Students needs mnemonic devices to face the understanding of new concepts, but they also need to be aware of the explanatory schemes behind mnemonic devices.

Table 2.1 Data extraction table used for our systematic review of the literature

The data extraction table was useful to highlight information available on 3 key-aspects:

- i) methodological aspects and didactic strategies
- ii) alternative conceptions;
- iii) main concepts that must be the subject of didactic transposition

The results of our survey are summarised in the following conceptual maps (Figures 2.1, 2.2 and 2.3), where the key-concepts on chemical bonding (placed in the foreground) are related to secondary concepts. These maps provide an overview of the focal points, problems and food for thought related to the main topic, at a glance. They also provide a kind of roadmap, useful for subsequent applications of these pieces of information.

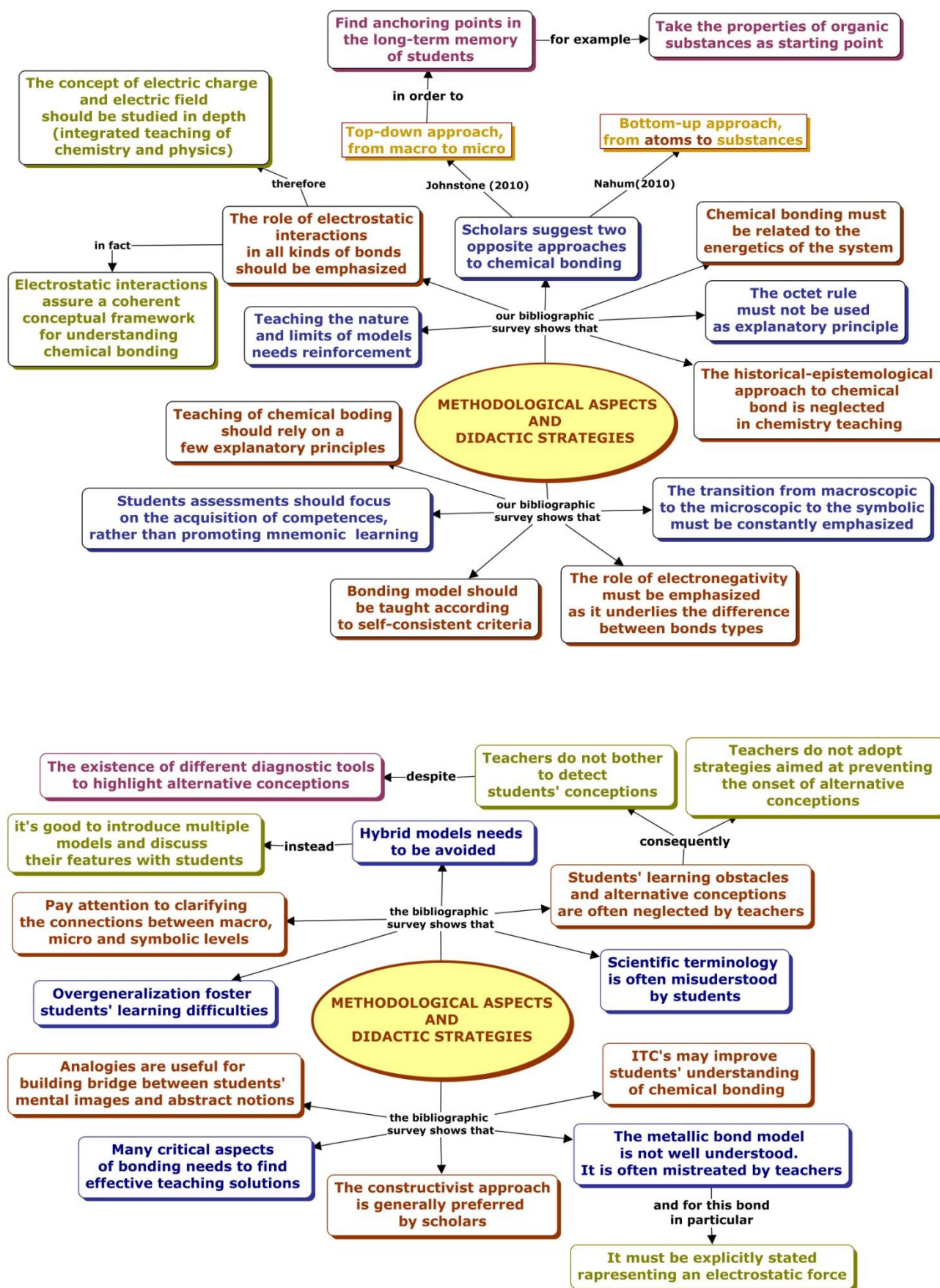


Figure 2.1 Concept maps related to methodological aspects and didactic strategies related the notion of chemical bonding

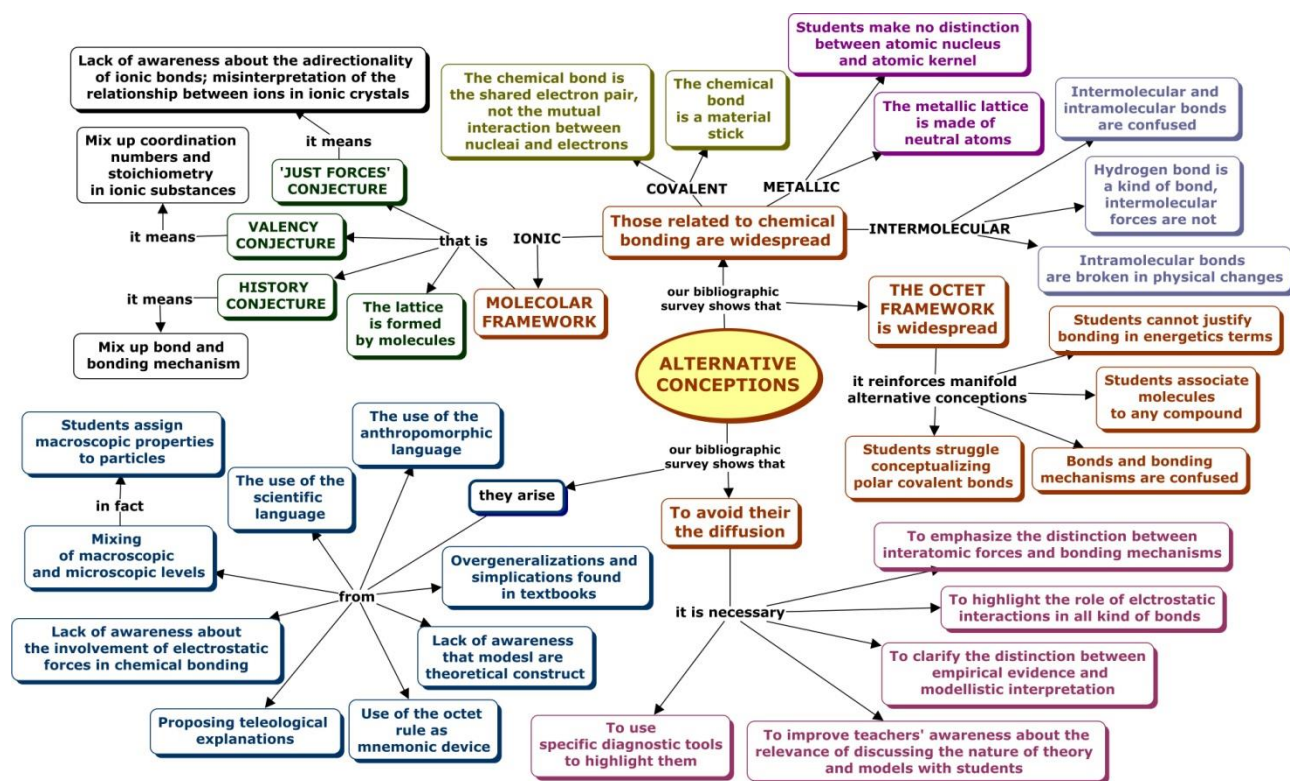


Figure 2.2 Concept map related to alternative conceptions related the notion of chemical bonding

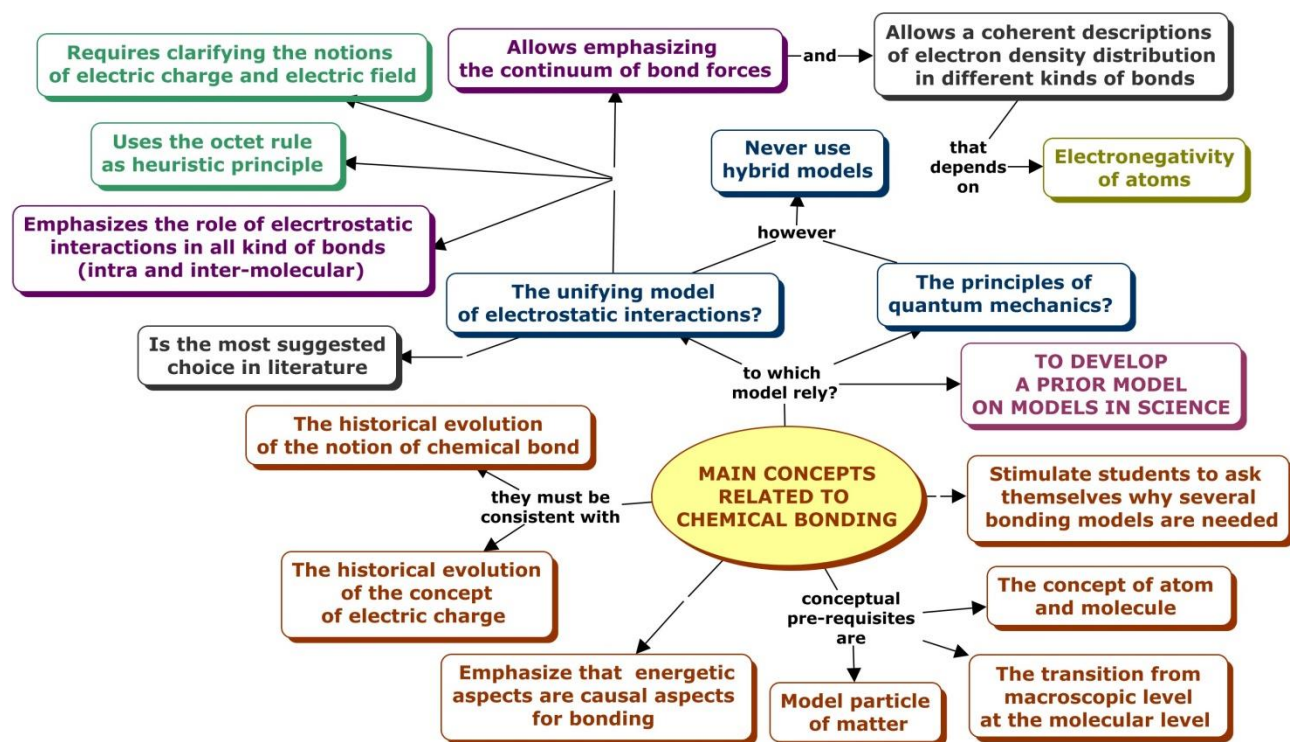


Figure 2.3 Summary of the main concepts⁵ related to teaching the notion of chemical bonding

⁵ The color code used in these maps have the sole purpose of making them more readable

2.2 Theoretical conceptual framework related to the teaching of the concept of interatomic bonding

A central problem of the didactic transposition of chemical bonding concerns the conceptual aspects inherent to this issue. Educational research in this field denounces the fact that chemical bonding is generally taught without inscribing the whole range of interatomic interactions into a rationalizing and unifying conceptual frame, grounded in a self-consistent conceptual context that relies on few basic principles (Levy Nahum et al. 2010, Joki and Aksela 2015 e 2018).

In most cases, chemical bonding is taught through a multiplicity of models, whose connection is rarely made explicit: this results in a fragmented and incoherent explanatory, that does not help students to grasp the relations of continuity existing between the different types of interatomic interaction. According to various experts, (Joki e Aksela 2015, 2018; Bergqvist et al. 2016), this unifying framework should be the reference to electrostatic or coulombian interactions, which are involved in the whole range of interatomic interactions. Joki and Aksela argue that this strategy prevents the emergence of different conceptions:

“To prevent alternative conceptual frameworks, different approaches in teaching chemical bonding have been presented [...]. The idea of the teaching model is to present electrostatic interactions as a common basis for all kinds of chemical bonding [...]. Our primary goal was to introduce electrostatic interactions as a basis for all types of chemical bonding before students adopt an octet framework” (Joki e Aksela 2018).

Only at a later stage will the different types of interactions be introduced, as a justification for the various range of macroscopic evidences (e.g. the difference between the properties of metallic substances and plastic materials). Bergqvist et al. argue that using a teaching model that emphasizes electrostatic interactions common to all types of bond turns out to be an intelligible model for students at a non-specialized school level; in addition, it prevents the onset of alternative conceptions and learning difficulties:

“This teaching model would be ‘at an optimal level of simplification’, i.e. kept as simple as possible *while still being scientifically correct*, thus providing a foundation for students to understand more sophisticated chemical bonding models based on quantum mechanics later on in their learning process” (Bergqvist et al. 2017).

This note is very important as it highlights that students’ understanding implies their ability “to assign meanings” to what they learn. Students manage to understand sophisticated bonding models only after been exposed to simpler (but scientifically correct) models: simpler models refer to phenomena and mode of description of the physical realm that are more familiar to students and therefore more understandable by them.

Obviously, this approach is not without criticalities. The same Joki and Aksela (2015, 2018) underline that the use of electrostatic attraction as unifying model has limits, in that it fails to account for the formation of electron pairs. Seemingly, the model of electrostatic attraction between opposite charges is challenged by the existence of biatomic substances made of two equal atoms. In fact, the attraction between species of opposite charge is somehow intuitive. Conversely, the formation of bonds between equal atoms is more difficult to justify and may be justified, in the first instance, by the interplay of attractions and repulsions between nuclear and electronic charges of both atoms involved. Besides, this is a conceptual problem that has been long debated by chemists, it was tackled by Lewis and finally solved by quantum mechanical models, as witnessed by the history of the notion of chemical bond (see Chapter 3).

The reference to the Lewis model, which is found in all school and university texts dealing with the chemical bonding, provides us with the opportunity to discuss its use in the didactic field. This model has the advantage

of being based on a few rules, which are clear and easy to apply. However, it is crucial not to give those rules an explanatory power that they do not possess.

Another critical point in the scholastic treatment of the chemical bond concerns historical-epistemological aspects. Epistemology and the historical development of concepts, despite their educational potential, are neglected in chemical education: the chemical bond is no exception. Ünal et al. (2006) criticize the fact that the historical-philosophical paths of the different scientific theories are absent in the chemistry textbooks. Joki and Aksela (2018) also claim the need for a greater awareness of teachers about the historical and epistemological background of scientific concepts. We agree with this remark; in fact, while designing the didactic sequence that is part of this thesis project, we have taken into account the historical evolution of the concepts of chemical bond and electric charge. The historical-epistemological approach that is typical of our research group supports the educational effectiveness of exploiting the conceptual knots that, historically, had to be addressed in the elaboration of a coherent model description of chemical bonding.

Many epistemological works on the chemical bond and related concepts can be found in the literature. For example, Croft and de Berg (2014) provide a contribution to the reconstruction of the history of the concept of chemical bond and electric charge. They state that looking at the historical development of three key-ideas (electric charge, octet and electron pairs) discourages mnemonic learning and hinders the onset of many common alternatives conceptions related to chemical bonding. Other authors (Yayon et al. 2012) stress the pivotal role played by the notion of electric charge in the understanding of the chemical bonding. Table 2.2 summarizes the knowledge related to charged particles that has to be borne in mind in order to understand electric phenomena related to chemical bonding.

Knowledge related to "charged particles"
Protons are positive
Electrons are negative
The charge of the nucleus equals the number of protons
In a neutral atom the number of electrons equals the number of protons
If the number of electrons differs from the number of protons, the atom is charged
If the number of electrons differs from the number of protons, the atom becomes an ion
Positive ions have fewer electrons than protons; negative ions have more electrons than protons
The partial positive or negative charge reported in the dipoles results from the fact that the electrons are mobile

Table 2.2 Knowledge related to "charged particles" relevant for understanding the notion of chemical bonding (Yayon et al. 2012)

This takes us to highlight the problem of the insufficient integration of the disciplinary teachings of physics and chemistry. Croft and de Berg (2014) emphasize that the concepts of electric charge and chemical bond are treated separately in physics and chemistry texts. In fact, physics textbooks deal with the concept of charge, but not tackle the problem of chemical bonding. The opposite happens in chemistry textbooks. Actually, these concepts should be tackled by both disciplines. In fact, the issue of chemical bonding is a privileged ground for intertwining the conceptual worlds of these two disciplines: a greater deal of interdisciplinarity in the teaching of chemical bonding, assured by a deeper integration of chemistry and physics teachings, would be beneficial to students' understanding of this phenomenon.

Another critical issue related with teaching chemical bonding concerns the ways the Lewis model is introduced, especially as regards to the octet rule. This rule is ubiquitous in the scholastic treatment of the chemical bond. Yet, Bergqvist and Chang Rundgren (2017) remark that it should not be used as explanatory

scheme, because the formation of chemical bonds is justified by the achievement of a minimum of potential energy by the system. So its final goal is not the generic achievement of an octet configuration:

“The ‘octet rule’ is a limited teaching model that students overgeneralise. Lack of discussion on why chemical reactions occur, frequent use of anthropomorphic explanations of chemical processes, and frequent use of the octet rule present feasible alternative explanations that fail to highlight that electrostatic forces contribute to all chemical bonds. This may result in an assumption that the octet rule is the reason for bond formation” (Bergqvist et al. 2017).

The energetic stabilization of the system as a justification for the formation of chemical bonds is not sufficiently emphasized by teachers and by textbooks. Joki and Aksela (2015, 2018) underline that the octet rule does not work, even when applied as mnemonic device (i.e. as a mental tool, able to systematize information, without any explanatory power). In fact, whenever a mnemonic device is applied without clarifying its explanatory background, it results in a poor and inconsistent conceptual structure. By conceptual structure, we mean a complex network formed by concepts, their features, mnemonic devices that connect concepts to each other, empirical evidences. Let's take, for example, the statement: "a metal and a non-metal form an ionic bond". This is a mnemonic device. An effective learning implies the presence of an explanatory scheme behind this statement: i.e., the formation of the ionic bonds should be justified on the basis of electronegativity gaps of the elements, ionization potentials and electronic affinities, which in turn are linked to the electronic configurations of elements.

According to Joki et al. (2015), effective explanations of chemical bondings do not simply oppose Coulomb interactions and the octet rule, plus considerations on stable electronic configurations. All this needs to be harmonized into a coherent explanatory frame. After discussing the explanatory principle of minimum energy, the octet rule can be introduced as a mnemonic device to estimate the combinatorial possibilities of atoms. For example, the fluorine atom has valence 1 because it needs an electron to get a full outermost shell, an event that leads the system to a more stable energy state as compared to the neutral atom.

2.3 Strategies and precautions for teaching and learning interatomic bonding

An essential didactic aspect related with the teaching of interatomic bonding concerns the sequence according to which the issues of chemical bonds and interatomic interactions should be addressed. Chemical bonding is traditionally approached by showing the classification of chemical substances into categories, that relies on the modeling description of different types of bond. This approach is schematized in Figure 2.4. The existence of different models of interaction (ionic, covalent, metallic) is anticipated by the classification of substances into those very same classes, according to an apodictic slant. In fact, these categories derive from explanatory models that have not yet been addressed; they are treated as if they were factual, rather than theoretical constructs rooted in modeling interpretations. In doing so, the levels of phenomenological evidence and modeling explanation are confused. This lays the foundations for misunderstanding both the notion of bond (and its correlates) and the procedural aspects of the scientific approach to reality. In the construction of scientific knowledge, the starting point is a phenomenological evidence, which raises problematic questions. The modeling activity comes later: it aims at finding plausible answers to those questions. By anticipating the classification of substances according to the categories derived from explanatory bonding models, the process is reversed and the problematic question underlying the whole process is cancelled.

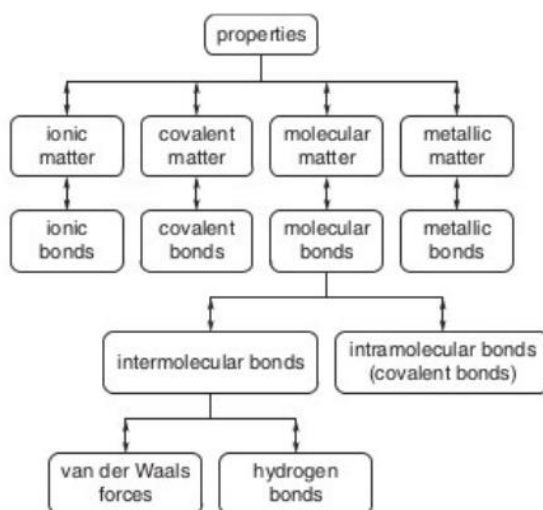


Figure 2.4 Schematic illustration of the traditional approach to the teaching of chemical bonding (Levy Nahum et al. 2008)

A second problem inherent to this practice is - according to Levy Nahum et al. (2008) - its rigidity. In fact, this approach is characterized by clean-cut definitions, that separates the different bond models very sharply, without highlighting their character of idealization (or, if you prefer, borderline cases):

“First, the presentation of each bond type as a different entity that belongs to a specific category does not foster a deeper understanding of chemical bonds. Specifically, it may obscure the important notion of *a unified rationalization of all chemical bonds based on underlying principles*. Second, over-emphasis of the four “ideal” categories is misleading and may actually hinder the learning process. While the “ideal” classification is not without merit, we now know that many important groups of modern materials simply cannot be “forced” into one of the rigid categories” (Levy Nahum et al. 2008, italics added).

Finally, this approach does not emphasize the continuum of bonding forces (shown in Figure 2.5), and helps fueling the alternative conception according to which the physical basis of intra- and intermolecular bonds is radically different. Conversely, highlighting the continuity between bond forces allows overcoming the rigid separation between types of inter-atomic interactions; it also emphasizes the idea that bonding is the result of a balance between attractive and repulsive electrostatic interactions, by using electrostatic interactions as a unifying principle:

“One of the key goals of the proposed framework is to stress that a continuum scale exists between extreme cases of qualitatively different bonding scenarios. Having understood, in stage 2, the common denominator of all bonds, we can now rationalize some distinct bonding categories, as shown in Figure 2.5” (Levy Nahum et al. 2008).

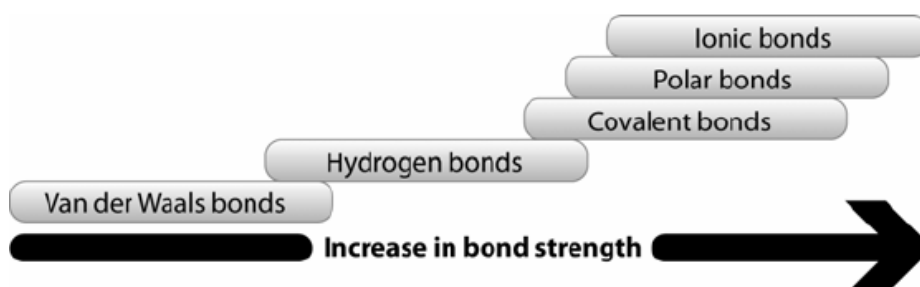


Figure 2.5 The continuous scale of bond forces (Levy Nahum et al. 2008)

The work by Levy Nahum et al. insists on the problems related with the distinction between inter- and intra-molecular bonds and the meaning of such distinction, which is different for physics and chemistry. This issue will be further discussed at the end of Chapter 3:

“First, it is important to understand that the traditional “intermolecular” versus “intramolecular” division, especially for hydrogen bonds, is superficial; if the relative scale of bond strengths is understood, one can understand that liquid water turns to gas by breaking hydrogen bonds even without this distinction. Second, it is essential to emphasize that *the transition between covalent-polar bonds and hydrogen bonds is blurred, rather than sharp*. Finally, it is also important to tell the students that many chemists prefer not to use the word “bond” for van der Waals interactions, as they prefer to reserve this term for *specific, directional interactions*” (Levy Nahum et al. 2008, italics added).

The aspect of directionality, which Levy Nahum assigns exclusively to covalent bonding, is relevant, albeit not diriment between the types of bonds: just consider that a typical ‘chemical’ bond, that is ionic bond, is not directional, whereas the inter-molecular interaction called hydrogen bond, has a marked directionality. Opposite to Levy Nahum's positions, Dhindsa and Treagust (2014) criticize the reference to the scale of bond strength shown in Figure 2.5, because the notion of bond strength is difficult to understand: “There are four limitations in this teaching approach: (a) the bonding concepts are arranged on the basis of bond strength – a concept that students find difficult to understand” (Dhindsa and Treagust 2014). Based on classroom experience, we believe that the notions of bond strength and bonding can be addressed in a didactically effective way. In our opinion, this scale cannot be disregarded as it allows introducing the topic of stability and lability of the whole range of inter-atomic interactions; furthermore, it seems to us that - once the role of electrons and electrostatic interactions is clarified – the scheme proposed by Levy Nahum helps highlighting that the distinction between different bond models is strictly related with the intensity of bond forces.

Another widely discussed issue in the literature is the sequence according to which different types of chemical bonding models should be introduced to students. Dhindsa and Treagust (2014) the most effective order follows the increase of bond forces, i.e.: pure covalent, polar covalent, ionic, metallic. Hence, they criticize the traditional sequence found in textbooks: ionic, pure covalent, polar covalent, metallic. According to these authors, the role of electronegativity in the formation of bonds should be emphasized: hence, the choice of proposing the above-mentioned sequential order. No doubt that the reference to electronegativity is a useful guideline for classifying inter-atomic interactions; nevertheless, this approach has limitations. For example, there are substances whose nature is different, despite a similar difference in electronegativity between the atoms that constitute them (e.g., sodium bromide NaBr and hydrofluoric acid HF, which are respectively classified as ionic and covalent, although the electronegativity difference is 1.9 in both cases). As for the relationships between bond strength and electronegativity difference, the example of metallic bonds is problematic, as metals are characterized by strong bonds and no electronegativity difference between bound atoms. Levy Nahum et al. (2008) point out this criticality: they remark that bond strength is determined by various factors (e.g. the atomic size). In fact, they exploit electronegativity differences exclusively in the discussion of polar covalent bonds, after a thorough description of ionic and pure covalent bonds based on other arguments. Electronegativity difference must be invoked while discussing the issue of ionicity percentage vs. covalent percentage in polar bonds (Dhindsa and Treagust, 2014; Levy Nahum et al., 2008). It remains that both the criteria to be applied for establishing the nature of a bond and the description of polar bonds in terms of mixed covalent and ionic bonds is not straightforward for the classroom.

Based on the number of critical issues discussed above, Levy Nahum et al. (2008) propose an alternative didactic approach grounded on the idea of a unifying principle for all types of inter-atomic interactions. According to the authors, this approach should prevent over-simplifications and improper generalizations.

This is the so-called "Bottom-Up" approach, shown in Figure 2.6. It exploits the single atom as the starting point and moves towards the justification of the properties of the substances, as its final point.

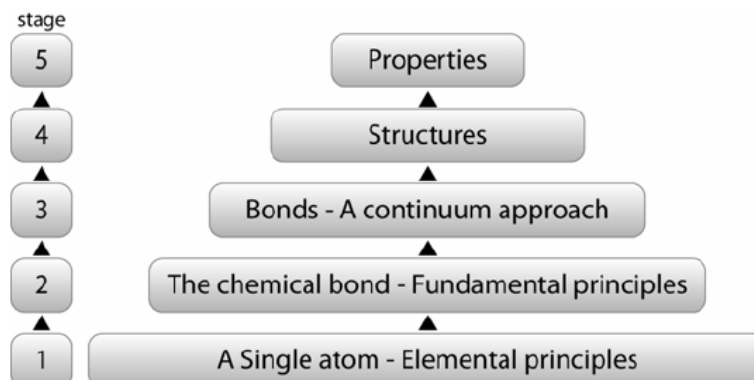


Figure 2.6 A schematic illustration of the 'bottom-up' framework for teaching the chemical bonding (Levy Nahum et al. 2008)

In summary, this approach implies five stages: the single atom and its properties represent the conceptual premise necessary to introduce Coulomb's law and the wave character of the electron. In fact, the authors choose not to present the electron as a material particle: they introduce the electron through the notion of orbital. The second stage answers the question "Why do atoms join together to form a chemical bond?". The concepts of energy and bond strength and their relationships are introduced here. This stage begins by considering that atoms attract each other due to electrostatic interactions established between nuclei and electrons of couple of atoms involved. The stability associated with the achievement of a minimum of energy is then introduced. All chemical bonds will therefore be characterized by a bond energy and bond distances determined by the balance between attractive and repulsive forces. In order to introduce these concepts, the graph of potential energy as a function of inter-atomic distances is introduced, as students need to understand the link between the chemical bonding and Coulomb's law. In the third stage, the ionic and pure covalent bonds are introduced and the continuity between the two extreme cases of chemical bonds is emphasized (Figure 2.5), by showing that the bond strength increases with polarity⁶. It is also emphasized that most bonds are partially covalent and partially ionic, i.e. polar. In this context, electronegativity is introduced as a parameter that helps quantifying bond polarity. This allows evaluating the asymmetric distribution of the electronic charge around the nuclei of bound atoms. Subsequently, intermolecular bonding is introduced. The fourth stage involves the explanation of molecular structures. The concepts of valence, periodic properties and VSEPR theory are introduced. Metallic substances are introduced as a peculiar case of covalent bond characterized by high electron delocalization. In the fifth stage, chemical bonding and molecular structure are connected to the properties of substances.

According to the authors, the "Bottom-up" approach allows preventing the main alternative conceptions on the chemical bond, which are fostered by the traditional teaching approach, whose limits are the following:

- The dichotomy between covalent and ionic bonds, which prevents understanding the continuity relationship between ionic and covalent bond models;
- The fact that electronegativity difference is used to distinguish between ionic and covalent substances, despite its limits. In fact, there are covalent substances whose elements display relevant electronegativity difference;

⁶ Incidentally, this emphasis can be a problem, as this is not true in all cases, as the tables showing the binding energies demonstrate.

- The fact that the octet rule is widely proposed despite the difficulty of reconciling it with everything that cannot be explained with the octet (atoms that do not comply with this rule, atoms with an odd number of electrons, the non-applicability of this rule to metal bonds or inter-molecular interactions). In fact, the octet rule is undoubtedly a useful guide but cannot represent the causal explanation for bond formation;
- The fact that the treatment of metallic bonds implies generalizations and over-simplifications. Generalizations comes from the fact that metallic substances are associated on the basis of few, common properties, without adequately highlighting the great differences among them. For example, ductility or resistance to corrosion can vary a lot from one metal to another. Simplifications lies in presenting metallic bonding as a lattice of “metal ions floating in a sea of electrons”, which has the effect of trivializing this model;
- The fact that intermolecular bonds are often described as "forces", as if their nature were different from that of so-called chemical bonds; it should instead be pointed out that these interactions share the same electrostatic basis with chemical bonds, but they are weaker and more labile. In addition, the different energies involved in distinct type pf bonding should not become a pretext for building a scale of relevance, as if chemical bonds were more important than inter-molecular interactions. Just think of their fundamental role in defining the properties of substances or their role. The rigidity of the traditional approach also comes out in talking about hydrogen bonding, which is predicated to exists only when oxygen, fluorine and nitrogen atoms are involve, whereas it may involve other elements, albeit resulting in weaker bond strength.

The "Bottom-Up" approach has interesting and shareable aspects, but it also shows some criticism. Its positive aspects are:

- It addresses the complex topic of chemical bonds under the unifying frame of electrostatic interactions; it also justifies bonding through energy stabilization arguments;
- It overcomes the sharp contrast between ionic and covalent bond by fostering the idea of the progressive increase of bond forces, from intermolecular bonds up to covalent and ionic bonds;
- This approach, based on the continuum of bond forces, allows presenting polar covalent bonds as hybrids between ionic and pure covalent bonding models.
- It clearly relates the properties of substances and materials to structure and bonding.

On the other hand, its problematic aspects are:

- The introduction of the principles of quantum mechanics at the high school level. In the first stage of their teaching scheme, Levy Nahum et al. (2008) avoid modelling the electron as a material particle, because they consider this analogy as misleading it would lead students to think of the attraction between nucleus and electrons as a sort of gravitational attraction, like the attraction between the Moon and the Earth. As a consequence, they prefer to present the electron as a wave and talk about electron density distribution around the nucleus. We disagree on this choice for various reasons. First of all, the explanatory effectiveness of this choice is not demonstrated. In addition, the introduction of the orbital notion at a sub-university level appears somewhat problematic, as it belongs to a theory (quantum mechanics) whose formal description implies the mastery of mathematical skills that are far from the learning objectives of secondary school students. There is a concrete risk of over-simplification, which may fuel alternative conceptions worse than those that one would like to avoid;
- This approach mixes different theories and models. In fact, electrostatic interactions are part of classical physics, whereas wave mechanics is not. So, Levy Nahum’s scheme refers to two theories of

completely different nature, despite the claim of making reference to a unitary explanation frame. We believe more appropriate to refer to a unitary theoretical framework and to develop models within a self-consistent frame. Furthermore, as Levy Nahum's scheme does not imply the description of bonding through valence bond theory or molecular orbitals theory, the need for introducing the wave character of the electron is not clear;

- The sequential order adopted by Levy Nahum for introducing various bonding models is the traditional one: ionic, pure covalent, polar covalent, hydrogen bonding and Van der Waals interactions. This is not fully consistent with the increase of bonding energies (from Van der Waals to the ionic bond) that Levy Nahum's approach wish emphasizing;
- The presentation of the bottom-up approach is extremely theoretical, as it lacks practical indications concerning how to practically implement this scheme in the classroom. In other words, clear indication concerning the didactic transposition of Levy Nahum's scheme are missing;
- The bottom to up approach, from atoms to substances, is very popular in chemistry texts, especially the more recent ones. Nevertheless, its didactic effectiveness is yet to be proven. Several scholars in chemical education (e.g., Johnstone 2010) have stressed students' difficulty to reconcile the macroscopic (phenomenological) level with the microscopic one (atomic and subatomic). In addition, the bottom-up approach risks to overshadow the problematic questions that foster the construction of explanatory models. Two main problem may result as a consequence of this approach: i) the procedural aspects of science are not highlighted to students; ii) student's curiosity is not stimulated. In our view, a condition for an effective didactic transposition is the manifest connection between chemical knowledge and the material world experienced by the students. The exploration of macroscopic phenomena in the first step is a crucial motivational factor; the building up of bonding model should respond to explanatory needs raised by such exploration.

In the light of these considerations, we believe that a didactic sequence on chemical bonds should adopt the macroscopic behavior of substances and the related problematic questions as the starting point. This approach is consistent with Johnstone's recommendations (2010): "Concepts must be built from the macroscopic and gradually be enriched with submicroscopic and representational aspects" (Johnstone 2010). In fact, problematic questions arise, at first, from the phenomenological (observable): seeking for explanations leads to atomic-molecular level, which is a modeling level. The connections between experimental evidence, microscopic interpretations and symbolic representations of phenomena (Johnstone's triangle in Figure 2.7) need to be built gradually. The relevance of making the interplay between the three explanatory levels of chemistry explicit to students is stressed by many scholars (Levy Nahum et al. 2010; Othman et al. 2008; Ünal et al. 2006): "Transitions between molecular and macroscopic representations as well as 'context shifts' when teachers switch between atoms and molecules in explanations, should be *explicitly conveyed* to students. These practices should be consciously used by chemistry teachers" (Othman et al. 2008, italics added). If students get used to recognize these relationships, this will help meaningful learning and contrast the onset of alternative conceptions. This is also Nelson's view, according to which students are introduced too early to the concepts of atom, molecule, electrons and ions; chemistry should instead be taught progressively: first come observations at the macroscopic level, then interpretation at the atomic-molecular level and finally at the electronic-nuclear level (Nelson 2002) according to the logical structure of chemistry (Jensen 1998).

The choice of effective explanatory schemes is crucial to didactic transposition. Nevertheless, Joki and Aksela (2015, 2018) remarks that the use of explanatory schemes for chemical bonding does not eliminate the practical need for mnemonic devices. However, mnemonic devices can feed fallacious ideas, if they are mistaken for explanatory schemes. For example, Tsaparlis, et al. (2018) report that the octet rule is often used

to predict whether the bond is ionic or covalent: in other words, it is improperly used as explanatory principle. In their daily teaching practice, teachers need to be aware whether they are using explanatory or mnemonic schemes; in fact, they need to make a balanced use of both (Joki and Aksela 2015, 2018).

Another typical problem related with the teaching of chemical bonding lies in the teleological use of the octet rule⁷ (Joki and Aksela 2015, 2018; Bergqvist, Drechsler and Chang Rundgren, 2016). This highlights the need for teachers to be trained in a greater awareness of the use of teleological explanations. Whenever the achievement of the octet is presented as a goal, the student loses sight of the real causes for bond formation, that is, the achievement of an energetically stable state by the system under study. Filling the outer electron shell is an effect, not a cause. Talanquer (2013) remarks that teleological explanations, which appear to be straightforward and simple, may become obstacle to a deeper learning as students get the illusion of having grasped the bonding concept:

“For many chemistry educators, anthropomorphizing atoms and molecules and *building explanations in terms of wants or needs (teleological explanations)* are useful pedagogical strategies for facilitating student understanding of abstract chemical models about the structure and properties of matter at the submicroscopic level. Nevertheless, teleological explanations generate an illusion of understanding that may hinder learning in the longer term” (Talanquer 2013, italics added).

Teleological explanations impair the student to seek deeper causal relationships: “This illusion of explanatory depth occurs because we are likely to confuse a superficial understanding of the consequences of processes (e.g., have a filled valence shell, gain stability, restore equilibrium) *for a deeper understanding of underlying mechanisms*” (Talanquer 2013, italics added). Nevertheless, even teleological explanations may be positively exploited to stimulate metacognition in students, by involving them in discussions aimed at highlighting strengths, weaknesses and criticalities of ineffective explanations. The development of metacognitive skills may foster analytical reasoning able to counteract the use of teleological explanations.

A further relevant and problematic aspect related to the didactic transposition of chemical bonding is the unaware use models that is often made in the classroom. Students often believe that the model is a proven fact, instead of a theoretical construct justified by a theory (Bergqvist et al., 2016). This may generate alternative conceptions, such as the transfer of macroscopic properties to microscopic particles. It is therefore essential to clarify that the foundational principles of chemical bonding are theoretical construct and not empirical evidence. This remark highlights some epistemic prerequisites essential to science teaching: i) the nature of models, their relationship with the material realm, their field of application should be clarified to students since the very beginning of the course; ii) students should be trained to distinguish perceptual facts from their explanatory models. Without these premises, the onset of alternative conceptions and the misunderstanding of the nature of scientific knowledge become practically inevitable.

Back to the teaching of chemical bonding, teachers should be aware of the impact of their own way of using models on student’s understanding. Whenever a bonding model is introduced, it is crucial to clarify its nature, its purposes and its limits, as well as its explanatory and theoretical character (Harrison and Treagust, 2000). The explanatory power of models has the potential to motivate students’ learning and clarifies the nature of scientific explanations. Unfortunately, textbooks often concur in fostering confusion and alternative conceptions, for example by proposing hybrid models (Bergqvist and Chang Rundgren, 2017). This is the case of the descriptions of the atomic structure that superimpose the iconographic representation of Bohr atomic

⁷ Tèlos is a greek term that means aim, purpose. A teleological explanation is an explanation that is constructed in order to justify *a priori* a given aim.

model and the verbal descriptions of electron density distribution or probability density typical of more advanced quantum mechanical models. Hence, teachers should make a critical use of textbooks, whose contents may be misleading and cause learning difficulties to their students. Unfortunately, many teachers have little awareness of the cognitive processes put in place by students in the interpretation of scientific models discussed in the classroom; these processes may inform on the onset of alternative conceptions. Hence the need for actively discussing analogies, metaphors and explanatory models with students. The arbitrary nature of models as reasoning tools also need to be highlighted:

“Teachers should, therefore, regularly check the students’ visualization of the analog in any metaphor, analogy, or model that they plan to use in class or which is found in the students’ textbook. Second, the analog-target mappings of all important metaphors, analogies, and models should be actively negotiated with the students [...]. Third, *the arbitrary nature of models and their use as thinking tools should be made explicit and this issue should be discussed in at least each content setting* [...]. Fourth, the legitimacy and desirability of multiple models should be introduced at an early stage and consistently developed and invoked during learning discussions” (Harrison e Treagust 2000, italics added).

The conventional nature of models, their being explanatory theoretical tools should be made explicit and discussed in the learning context. The legitimacy and desirability of multiple models should be constantly reaffirmed and shared with students: in fact, learning an informed use of models should be a constant practice in the classroom, opposite to mnemonic learning of textbooks’ content, as part of a true scientific practice.

Teachers should also be aware of the evolution of their students' mental models, i.e. the representations and meanings that students associate with the models they learn. Useful practices are: to invite students explaining the meaning of a model; to propose problem-solving situations based on the use of models; to allow students using, manipulating, applying and comparing different models. Teachers able to identify the *zone of proximal development*⁸ of their own students will be able to judge when students can be exposed to new models, in order to maximize learning.

It has also to be borne in mind that the use of models is different by experts and beginners (Coll and Treagust, 2002, 2003). Experts are well aware that a model must meet the user’s needs, therefore it can be modified: hence, experts make a pragmatic use of the model. The same is not true for students, who obviously lack experience and practice.

In chemistry, most models are representations of the microscopic realm aimed at interpreting macroscopic behaviors or properties. Models are often derived from other models: for example, molecular models derive from the particle model of matter.

Using several different models referred to the same content improves students’ conceptual understanding of students. Models’ features and limits must be explicitly discussed with students, so to lead students to a better understanding of the function and use of models. According to Ünal et al. (2006) students exposed to multiple models attain a better comprehension as compared to students who focus on a single model, albeit the most refined:

⁸ The zone of proximal development is a concept introduced by the Russian psychologist Lev Vygotsky (1896-1934) and is defined as the distance between the current level of development and the level of potential development, i.e. what can be achieved with the help of other people, either adults or peers with a higher level of competence. According to Vygotsky, the educator should propose to the learner problems of a level a little higher than his current skills, but still simple enough to be understandable. Being familiar with the concept of "proximal development zone" offers the opportunity to reinforce the learner's learning process, instead of hindering it, thus preventing any sense of frustration and failure.

“There are several reports of ways of enhancing students’ understanding of chemical bonding. It seems that using multiple models including analogies helps students understand that models are just that, models of a reality we cannot ever see. [...] Similarly, *students who were encouraged to use multiple particle models displayed more scientific understandings of particles and their interactions* than did students who concentrated on a ‘correct’ or best analogical model” (Ünal et al. 2006, italics added).

The necessary premise is that teachers make appropriate use of models otherwise alternative conceptions may arise. The limits of each models and the definition of its field of application must be clarified to students.

Let’s go back to discussing teaching problems that are specific to the notion of chemical bonding. Here is a list of teaching practices and verbal expressions that may generate learning difficulties (Bergqvist et al. 2016):

- Anthropomorphic descriptions are widespread and consists in assigning human attributes to chemical objects: e.g., expressions like "Atoms are hungry for electrons", "Atoms desire electrons", "Electrons share as brothers", "Atoms are jealous";
- The formation of various types of chemical bonds is presented as a result of the interaction between single isolated atoms: chemical bonding is not contextualized in the reaction environment. Typically, the formation of NaCl implies the interaction of a single sodium atom and a single chlorine atom. In doing so, the formation of an ionic lattice becomes difficult to justify;
- Ionic bonds are presented as a result of electron transfer events aimed at satisfying the octet rule (teleological explanation of the octet) instead of focusing on the energy stabilization of the system and ion formation. As a result, students may identify ionic bonding with electron transfer instead of the electrostatic forces that keeps ions together (Bergqvist et al. 2016);
- Lack of use of the graph of potential energy as a function of interatomic distances (Lennard-Jones potential) in order to discuss the driving force for bond formation;
- The term ‘electrostatic force’ is rarely used. The most common term is ‘attractive force’: hence, charge repulsion is overshadowed. In general, the interplay between electrostatic attractions and repulsions in the formation and stabilization of chemical bonds is little emphasized. For example, according to Bergqvist et al. (2016), covalent bonding is rarely presented as a dynamic event that involves electrostatic forces, it is often conceived as a static pair of electrons: “regarding covalent bonding, the conception that the shared electron pair in itself is the bond, and the electron pair holds the atoms together because they then get noble gas shell”.

In fact, the role of the interplay of electrostatic attractions and repulsions among subatomic components should be emphasized in discussing the general phenomenon of chemical bonding: this would help students to spot out all the actors involved in bonding, instead of simply memorizing electron transfer or sharing.

A difficult type of bonding model to be discussed in the classroom is the metallic bonding model. According to Cheng and Oon (2016) it is essential to stress its character of electrostatic force joining the electrons of the external atomic shells and the cores (nucleus + electrons of the internal shells) of metal atoms. This would impair the onset of alternative (Bergqvist, 2016). Lexical and iconographic choices made by teachers are especially critical in the treatment of this type of bond mechanism.

Finally, we would like to briefly discuss the role of ICT’s in teaching chemical bonding. The use of digital tools may improve both students’ comprehension and interaction (Patron et al. 2017; Frailich et al. 2009). Learning activities may become more engaging and stimulating, thanks to the use of visual representations and web tools like animations, simulations, modeling softwares, interactive games. These tools may improve

the active role of students in the learning process and they may improve students' interaction with peers and the teacher. Peer learning is favored by online activities carried out in small groups. As for the conceptual aspects, dynamic representations of the atomic structure are more effective than 2D static images, as they help students' understanding of the dynamic character of microscopic particles. In some cases, the use of ICTs helps understanding the relation between the macroscopic and the microscopic levels of chemistry. It may also help students verify the limits of each model and the relationships between distinct models, thus getting a more realistic notion of what a model is and what it is for. In general, the use of technologies feeds students' motivation, given the central role they play in their lives: their careful use may favor a student-centric rather than teacher-centric teaching approach. According to Frailich et al. (2009), the use of ICTs would even favor the constructivist approach.

Nevertheless, it is important to keep in mind that technological tools are just tools: they can assist the learning process, but they cannot replace the teacher's action, nor they represent innovative teaching strategies *per se*. In addition, they may hide dangerous traps related with the communications codes employed by these tools. So, it is essential that the communication codes related to model representations are made explicit, shared and discussed with students, in order to avoid misunderstanding between the teacher and students:

“Iconographic and symbolic languages rely on communication codes, just like natural language. Whenever these codes are not made explicit and shared with students, i.e. *whenever teachers assume that students spontaneously assign the same meaning to signs and symbols as teachers do, then teachers set the stage for dramatic misunderstandings*. So, iconography may become a vehicle for alternative conceptions and poor comprehension, that is a learning obstacle”. (Ghibaudi 2019, italics added).

Students need to be trained at a critical exercise towards visual representations:

“First, we argue that chemistry teachers need to be aware of the challenge that students may experience when trying to make meaning of visual representations. Second, they need to be able to problematize and reason about their use of visual representations, why a certain representation can be more or less appropriate than another in a certain context, and how representations can be varied in ways that provide optimal possibilities for the students to access the needed discernment” (Patron et al. 2017, italics added).

Without a proper training of students and a critical reflection by the teacher about the tool to be used and the aim to be achieved, ICTs are not helpful. They may even become source of alternative conceptions. For example, they may lead students to confuse models with the real world, to assign macroscopic properties to microscopic entities (e.g. the color of an atomic nucleus, represented as a ball), or to give a wrong interpretation of symbols and signs (e.g. to take electron orbits as if they were material paths). In fact, ICTs for chemistry rely on visual representations of the atomic and subatomic worlds, which are, in themselves, not representable, as they belong to the quantum world. Teachers need to be well aware of this intrinsic contradiction in order to avoid fostering misconceptions. This requires a high degree of epistemological awareness by teachers:

“Furthermore, by familiarizing themselves and discussing research in this area, we believe teachers would come to appreciate the affordances and challenges associated with the use of visual representations. In line with Bergqvist et al. (2016), we also argue that *it is essential that practicing teachers are given the opportunities and the support to think about their use of representations, both on their own and with their colleagues*. These issues should be important to address not only for teachers in chemistry but also for science teachers in general, since many parts of science are

concerned with phenomena that are complex or not directly visible” (Patron et al. 2017, italics added).

Therefore, the conditions for an effective use of ICTs are that teachers operate informed choiced about the tools to be used and they discuss with students both the teaching aims of such activities and the communication codes exploited by ICTs, must always stimulate reflection on each proposed content.

2.4 Cognitive/pedagogical aspects

The learning process depends on the activity of the learner (constructivist model) and on the pedagogical context, i.e. on all those teaching practices aimed at promoting understanding rather than the mnemonic acquisition of contents. In order to achieve this goal, teachers should be aware of the subject’s cognitive processes involved in knowledge costruction and take them into account in their teaching choices (e.g., when deciding the appropriate level of conceptualization to be proposed to students). This section deals with the issues pertaining these two crucial areas.

As regards to the level of conceptualization, we have already mentioned that several scholars (Joki et al. 2015; Levy Nahum et al. 2008 and 2010; Dhindsa and Treagust 2014) put into question the opportunity to introduce quantum mechanics concepts to address the topic of chemical bonding at the secondary school level. In fact, secondary school students cannot handle the cognitive and mathematical tools needed for understanding and formalizing abstract concepts such as atomic orbitals. The result is that these concepts are proposed in a simplistic and non-rigorous way, thus inducing alternative conceptions (e.g., the identification of orbitals with space regions to be filled in with electrons) that are difficult to eradicate in subsequent school contexts. In order to get a real comprehension, students need anchor new concepts to their own experience and knowledge, in a constant process of revision of their own conceptual process:

“Learning is therefore understood as a process of development of the subject which consists in finding an agreement between one's own logic and the logic of the knowledge (to be learnt): hence *a conceptual change is impossible without a contextual restructuration of the learner’s structures of knowledge and conceptual networks wherein a concept acquire a specific meaning*. It is a process that is not immediate and follows a spiral path, along which those very same concepts are gradually constructed at increasingly higher levels of complexity, in order to adapt to the increasing cognitive abilities of students” (Roletto 2005, italics added, my translation).

Therefore, there must be a correspondence between what students are able to understand at a specific stage of their cognitive development and what the teacher proposes, in terms of the content to be learned and the formalization of such content. This implies the graduality and recursiveness of the learning process, that allow a progressive, increasing degree of generalization:

“Scientific concepts cannot be assimilated once and for all and in a final form; *the construction of concepts takes place progressively, in the course of a development that passes through different registers or levels of conceptualization, gradually more formal and more general*. The idea of a conceptualization register implies a spiral path for teaching and learning concepts; in some cases, this path retraces the steps through which formalized knowledge was developed. This cannot be done mechanically, It rather *requires an accurate didactic transposition* in which, on one hand, one needs choosing the conceptualization level which is more appropriate to the cognitive abilities of students; on the other, the transition from one level of conceptualization to another one always implies a restructuration of its own conceptual networks” (Roletto 2005, italics added).

Didactic transposition is therefore the action that decides the effectiveness of the teaching practice: only an accurate transposition, consistent with the cognitive level of those to whom it is addressed can hope generating an authentic understanding. One aspects that must be taken into account by the didactic transposition of chemical bonding is its consistency with the current scientific and pedagogical knowledge. Some authors have developed targeted proposals for this purpose. Evidence that university professors prefer using few unifying fundamental principles and to highlight the complexity of the theoretical-conceptual framework of chemical bonding is reported by Levy Nahum et al. (2007). These authors report radically distinct views of university and high school teachers, respectively, as regards to how chemical bonding should be taught: the formers stigmatize the excess of simplification and conceptual stiffness in the didactic transposition of chemical bonding made at school; conversely, the latters claim the need for clear definitions and rigid classifications:

“It is very difficult to teach the “gray” zone of chemistry. The teacher must first present the facts clearly and must teach the “black and white” zones. The first step of teaching must be dichotomous: teaching the two extremes, first ionic/covalent bonds, and only later breaking them apart and reorganizing students’ knowledge. [...] We need to simplify things and provide students with generalizations and rules because chemistry must be presented as an exact science.” (Levy Nahum et al. 2007).

On the other hand, both categories agree on focusing on electrostatic interactions and stressing the relationships of continuity between different types of bonds. They also underline the didactic usefulness of the potential energy graph.

Another relevant problem is the choice between the *bottom-up* or *top-down* approaches. We already mentioned Johnstone’s doctrine (2010): he claims the pedagogical appropriateness of using macroscopic phenomena as the starting point for teaching chemistry (Figure 2.7). Interestingly, according to Johnstone, chemical bonding could well work as a bridging notion between the macroscopic and the microscopic realm. In fact, even if atoms and molecules are inaccessible to senses, the properties deriving from their interactions (i.e. from chemical bonding) are easily observed in substances (e.g. color, physical and mechanical properties, reactivity, etc.).

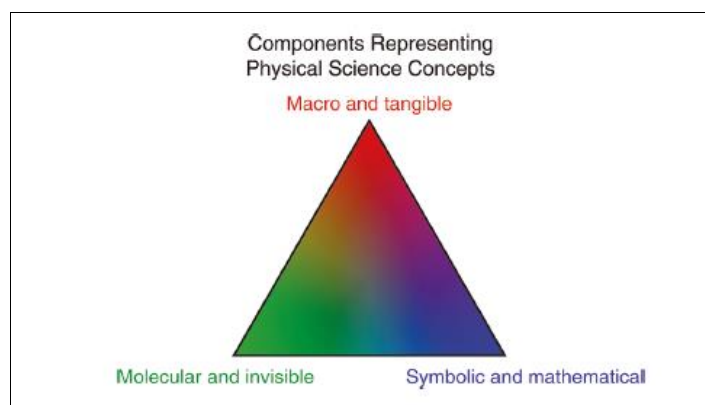


Figure 2.7 The three levels of chemistry according to Johnstone (Johnstone 2010)

Among other reasons, this choice would allow building up anchor points in students’ long-term memory. Johnstone refers to Ausubel et al. (1978) according to which the subject selects external stimuli based on his own interests and on what he is able to give meaning to. These preventive choices act as a filter:

“In effect, we each have a unique filter by which we individually select what interests us, what makes sense to us, and what is important to us”. (Johnstone 2010).

The relationship between learning mechanisms and memory is also discussed by Pascual-Leone, Case, and Scardamalia (Case 1985) who rely on the concept of *working memory* (Figure 2.8), according to a functional

conceptual approach. The working memory can receive new pieces of information, but may also retrieve information from long-term memory (Baddeley 1986). In the working memory, various pieces of information interact to establish connections between the new and old knowledge. Sometimes these connections generate alternative conceptions, sometimes connections are not created at all and information is rejected or mnemonically acquired. According to these authors, working memory reaches its maximum potential at the age of sixteen. The greater the extent of working memory, the greater the ability to support complex reasoning. An advantage of this view is consists in highlighting the risk of cognitive overload. According to this learning model, many learning difficulties are related to excessive informational load, especially for beginners, with the risk that their working memory goes haywire. Clearly this model refers to a cognitivist learning view, where the learner is compared to an information processor: this learning view is far from constructivism (which inspires the present work) refers and is equally distant from Johnstone's positions. However, the reference to memory storage mechanisms may be useful.

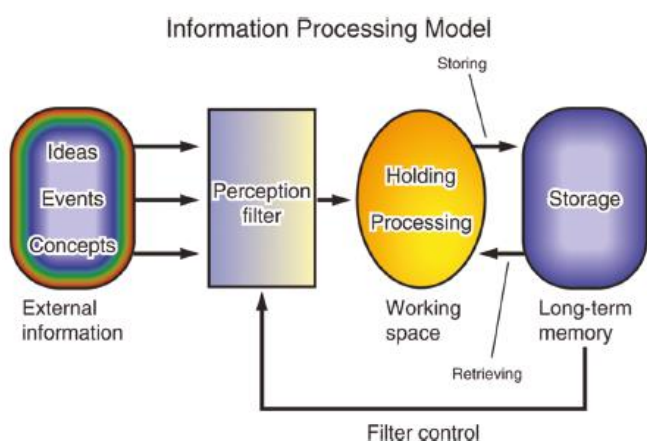


Figure 2.8 Schematic model of learning deriving from Piaget's disciples view (Johnstone 2010)

In fact - going back to Johnstone's view - if the starting point of didactic transposition are abstract contents (such as the electronic structure of atoms, the principles of chemical equilibrium separated from the related phenomenology, etc.), the links in long-term memory are likely missing and learning becomes purely mnemonic. Dhindsa and Treagust (2014) remark the need to start from where students are: this allows supporting students' own interests and experiences, leading them to develop new ideas related with those already familiar to them. Other caveat for an effective chemistry teaching are, according to Johnstone:

- ✓ Avoid teaching anything that will have to be demolished later;
- ✓ Avoid oversimplifications, which can lead to future obstacles;
- ✓ Avoid over-compressed learning time-schedules.

Setting a proper teaching schedule is essential for the learning process to be effective and incisive.

We already discussed the central role of models in teaching chemical bonding. The cognitive aspects of learning are fundamental in this area: students exposed to scientific models develop mental representations of such models. These are related with students' cognitive sphere and provide valuable information on the conceptual structure of students (Coll and Treagust 2003).

Harrison and Treagust (2000) remark the distinction between analogical models and mental models. Analogical models are models that share well identifiable attributes with their own object of study (or theory). Analogical models refer to the concrete, abstract or mixed representation of scientific concepts. In chemistry, analogical models can be molecular models, chemical formulas, but also mathematical models such as the ideal gas law. Conversely, mental models are specific types of mental representations generated during the

use of cognitive functions. They are functional systems in evolution, that is, they have no clear boundaries and are incomplete: they are personal and very difficult to be unmasked. They serve as mnemonic devices to aid memorization and to predict the behavior of physical systems (Harrison and Treagust, 2000). Mental models, according to Coll and Treagust (2003), are divided into physical and conceptual: the physical ones represent the physical world, the conceptual ones represent abstractions. "Synthetic mental models" may also exist: they represent the evolution of alternative concepts due to the interaction with scientific concepts (Harrison and Treagust 2000). Both analogical and mental models are conceptual entities that serve to satisfy an explanatory need, so from this point of view they are similar.

Analogical models are attractive to students and teachers, as they allow the abstract world of concepts to be traced back to familiar and everyday objects and to common sense concepts, but it is precisely this aspect that makes analogical models a double-edged sword. Generally, learners oppose resistance to changing their own mental schemes (Coll and Treagust 2003): they tend, at first, to keep common sense conceptions; subsequently, they tend to replace them with simple or simplistic interpretations (models) instead of taking on more elaborate and more effective ones:

“The learners do not see the need for an explanatory theory as powerful as the scientific one and thus are satisfied with their own less powerful theory, despite the fact that these theories or mental models do not take into account some limitations of their models” (Coll and Treagust 2003).

As regards to chemical bonding, this may result in conceiving interatomic bonds as material connections instead of interatomic forces; or in thinking of metallic bond as a "sea of electrons" instead of going for more accurate description. The two types of models interact to become a concrete operational model that allows dealing with new and old ideas. When a student listens to his teacher, he studies a textbook or watches a simulation, the proposed analogical model meets its own mental model and the interaction is influenced by many variables (Harrison e Treagust 2000). In fact, the interpretation of the analogical model depends on the student's previous knowledge, ways of thinking and linguistic competence. The way in which a student interprets and assimilates a model is unpredictable since the construction of knowledge is a personal fact and access to the mental models of others is difficult. Coll and Treagust (2002, 2003) remark that (analogical) scientific models never coincide with the students' mental model: therefore, teachers should verify how students learned a model and how they master it. Coll and Treagust (2002, 2003) show that there are inconsistencies between the models proposed by teachers and mental models used by students for interpreting metallic and covalent bond models.

Students' alternative conceptions unveil alternative (and apparently satisfactory) pseudo-explanations for various phenomena: these conceptions are not necessarily evident to teachers, as they can be hidden in the folds of apparently consistent answers (e.g. answers to a test). There is also a motivational barrier: students do not feel the need to improve their mental models with better models, because they are in many cases satisfied with the explanations they are able to give. Furthermore, students do not always completely get rid of the earlier and simpler model. For example, the model of the metallic bond as a "sea of electrons" is very popular because the key feature of electron mobility justifies many properties. Instead, the students' preferred mental model for covalent bond is based on the octet rule and the stability of full electron shells. The mental models of undergraduates and graduates are obviously more sophisticated than those of high school students: nevertheless, it is well established that even university students exposed to very sophisticated models tend to mentally retain the most simplistic explanatory models. This highlights the importance of building learning paths that maintain their coherence along the path from school to university: otherwise, the risk that university students are negatively affected by their previous knowledge and alternative conceptions is high.

Finally, it should be borne in mind that using advanced scientific models (such as quantum mechanical ones) implies the ability to use formal thinking at a level inaccessible to high school students (Coll and Treagust 2003). In fact, teaching highly abstract models at school is judged counterproductive by several researchers such as Gillespie, Spencer and Moog (1996a, 1996b), Ogilvie (1990), Bent (1984) and Weinhold (1999).

2.5 *Alternative conceptions*

A central problem in chemical education is represented by students' alternative conceptions (Figure 2.2). These can be fueled by inadequate didactic transpositions. This topic is widely discussed in the literature (Levy Nahum et al. 2010; Cooper et al. 2015); Schmidt et al. 2009): it includes repertoires of alternative conceptions, hypotheses about their origin, diagnostic tools to highlight them and didactic suggestions for preventing their onset. Table 2.3 summarizes the most significant alternative conceptions reported in the literature on the subject of chemical bonding (and some related concepts).

Alternative conceptions		References
Intramolecular bonds	The idea that a polar covalent bond has a partial ionic character leads to believe that this bond involves the presence of ions	Tsaparlis, Pappa, and Byers 2018 Coll and Taylor 2001
	Ionic compounds are made up of molecules	Tsaparlis, Pappa, and Byers 2018 Ünal et al. 2006 and references therein Coll and Taylor 2001 Othman, Treagust, and Chandrasegaran 2008
	Coulombians forces are exclusively involved in ionic bonding	Tsaparlis, Pappa, and Byers 2018
	Covalent bonding coincides with electron sharing: electrostatic attraction between nuclei and electrons is neglected	Ünal et al. 2006 and references therein
	Ionic bonding coincides with electron transfer: electrostatic attraction between ions of opposite charge is neglected	Levy Nahum et al. 2010
	Electron configurations determines the number of ionic bonds that may be formed.	Ünal et al. 2006 and references therein
	The breaking of a chemical bond results in energy release	Ünal et al. 2006 and references therein

	Covalent bond is a weak bond	Othman, Treagust, and Chandrasegaran 2008
	Metals are made up of molecules	Ünal et al. 2006 e and references therein
Intermolecular bonds	Intermolecular bonds involves atoms within a molecule	Peterson and Treagust 1989
	Hydrogen bonds are stronger than covalent bonds	Ünal et al. 2006 and references therein
	Covalent bonds break when a substance changes its physical state	Ünal et al. 2006 Schmidt, Kaufmann, and Treagust 2009 Othman, Treagust, and Chandrasegaran 2008
	Strong intermolecular forces are displayed in covalent solid lattices	Ünal et al. 2006 and references therein
	Ionic and metallic bonds are examples of intermolecular interactions	Coll and Taylor 2001
Bond polarity	Bond polarity depends on the number of valence electrons of the atoms involved in the bond	Ünal et al. 2006 and references therein
	The polarity of the bond determines the shape of the molecule	Peterson and Treagust 1989
Molecules' polarity	Molecules are polar whenever they contain polar bonds	Ünal et al. 2006 and references therein
	Molecules are non-polar whenever they contain atoms with similar electronegativities (there is no connection between molecule's polarity and structure)	Peterson and Treagust 1989
Molecular shape	The shape of a molecule is only due to the repulsion of bonding electron pairs	Peterson and Treagust 1989
	The shape of a molecule is only due to the repulsion of non-bonding electron pairs	Peterson and Treagust 1989

	Bond polarity affects molecular shape	Peterson and Treagust 1989
	The shape of the molecule depends on the number of atoms bound to the central atom of the molecule	Erman 2017

Table 2.3 Some common alternative conceptions on chemical bonding reported in the literature

A recent work by Tsaparlis et al. (2018) carried out on Greek students, coming either from university or high schools, shows that a diffuse alternative conception on chemical bonding consists in taking into account only attractive forces and neglecting repulsions: “It would appear that most students associate the concept of bonding only with attractive forces, and therefore ignore the repulsive forces (electron-electron and nucleus-nucleus repulsions). Clearly, this finding suggests that this likely misconception needs to be carefully considered when teaching chemical bonding” (Tsaparlis et al. 2018). Another common mistake is to confuse inter- and intramolecular bonding, due to the similarity of these two terms (Ünal et al. 2006; Peterson and Treagust 1989). Actually, this is a clear sign that many students do not realize that these interactions rely on distinct mechanisms. In fact, students are reported to believe that inter-molecular bonds are found within the molecule or within ionic or metal lattices; in addition, they do not pay attention to the magnitude of bond strength in these two classes of inter-atomic interactions. Coll and Taylor (2001) report that students understand the relationship between inter-molecular forces and boiling points, but they still believe inter-molecular forces to be stronger than intra-molecular ones. According to Coll and Taylor (2001), bond strength in ionic, metallic and covalent substances is perceived as weak, despite macroscopic evidence like the hardness of metals. For example, ionic bonds are believed to be weak based on the fragility of salt crystals:

“The view that the electrostatic forces holding ionic compounds together are weak also was prevalent. This view was *the most common explanation offered by the students for the friability of ionic salts* such as sodium chloride that was depicted in focus cards and was evident across all levels of student from secondary school to postgraduate” (Coll and Taylor 2001).

The list of alternative conceptions on chemical bonding is rather long: electronegativity is often understood as the attraction of a single atom towards a single electron, so this notion is not contextualized in the frame of chemical bonding. The relationship between electronegativity and bond polarity seems to be an obstacle, as well. Seemingly, the relationship between molecular polarity and structure is often unclear: many students believe that non-polar molecules must contain non polar bonds; others believe that molecular polarity is determined by valence, lone electron pairs or ion charge (Coll and Taylor 2001). The connection between chemical bonding and electrostatic phenomena is often unclear. The idea of electron mobility and its logical consequences seem to be especially difficult for students to understand. Electrons (and charges) are often imagined as localized and static. Thus, polar molecules are believed to contain charged species and the formal notion of partial negative charge is confused with that of ion.

Metallic bond is especially challenging for students: metal lattices are reported to be made of neutral atoms or even molecules. Surprisingly, these conceptions are found even among undergraduates and graduate students who have already been exposed to general chemistry courses (Coll and Taylor, 2001).

Several alternative conceptions on chemical bonding fall within the so-called Molecular Framework, a classification elaborated by Taber (1997), which is opposed to the canonical Electrostatic Framework. The main idea of the Molecular Framework (summarized in Figure 2.9) is that, in ionic lattices such as sodium chloride, each ion does not interact equally with the other six ions that surround it. The lattice is thought as if

it was made of ion pairs corresponding to the formula unit NaCl. The formula unit is therefore thought of as a molecule, within privileged interactions between pairs of atoms.

According to Taber, several conjectures concur in building up the Molecular Framework: the Valency Conjecture, the History Conjecture, and the 'Just Forces' Conjecture.

The Valence conjecture links the electronic configuration of ions with the number of ionic bonds that ions may form (e.g., the sodium atom gives up just one electron, therefore it forms a single ionic bond with a chlorine atom).

The History conjecture considers that neutral atoms are invariably the starting point for bond formations. For example, sodium chloride is always the result of a reaction between a neutral sodium atom and a neutral chlorine atom, who undergo electron transfer. So, according to this conjecture, sodium chloride cannot be the result of an exchange reactions between ionic substances such as, for instance, sodium nitrate and potassium chloride.

The “just-forces” conjecture consider that, in the ionic crystal lattice, ionic bonding involves two ions next to each other, whereas their interaction with the other ions in the lattice is due to unspecified forces, that cannot be qualified as ionic bonds.

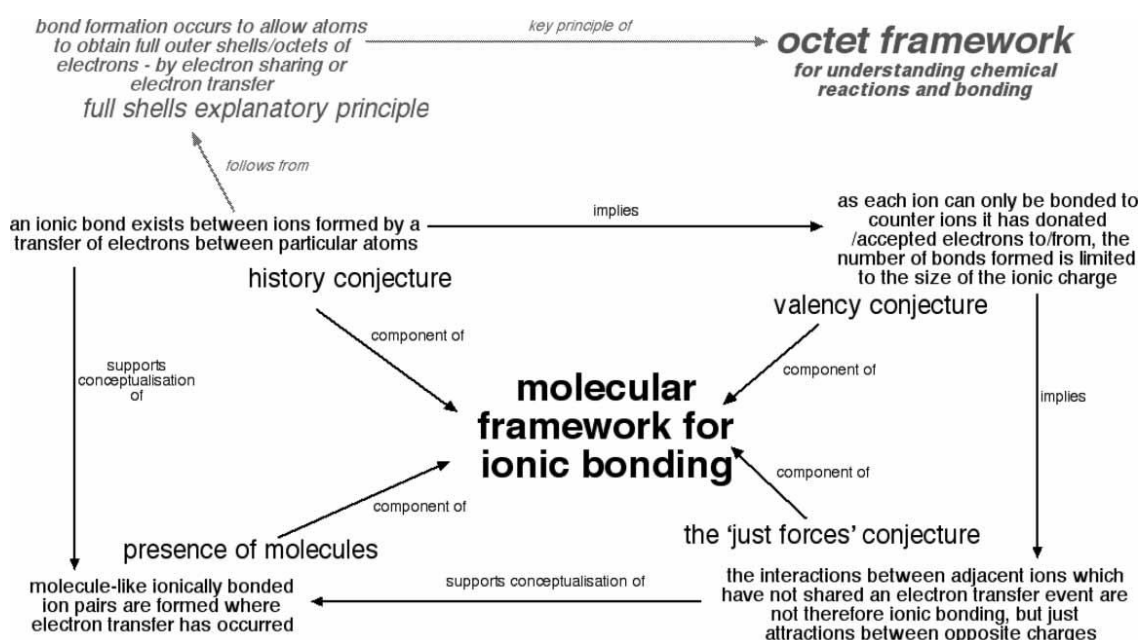


Figure 2.9 An alternative conceptual framework for ionic bonding representing the thoughts of English college students (Taber et al. 2012)

The Molecular Framework reflects the way of thinking of students who emphasize the transfer of electrons, associate the chemical formula of the ionic compound with the molecule and have an inappropriate idea of valence. Taber's thesis is supported by Vladošić et al. (2016), who argue that the ionic bond model is not well understood by both high school and university students, and even by a non-negligible number of teachers.

According to Taber, this is the result of a common teaching practice: ionic bonding is usually presented as the result of electron transfer between two neutral atoms, instead of being identified with the Coulombian interaction between ions. This is History conjectured, fostered by many textbooks which emphasize the formation of ions and leads students to believe that:

“Ionic bonding is formed as a result of an electron transfer, and a bond is formed between the donor and the acceptor in this process. There is an obvious source of this misconception in textbooks. Almost without exception, the section on ionic bonding is introduced via a discussion of

the formation of a positive ion and a negative ion by electron transfer, usually between a sodium atom and a chlorine atom” (Vladušić et al. 2016).

In fact, it is customary to show the mechanism of ion formation and subsequently provide examples of various stoichiometric combinations of ions in different ionic substances.

Nevertheless, we do not fully agree with Taber’s position, both on the theoretical and didactic viewpoints. From the theoretical side, we believe that focusing exclusively on Coulombian interactions, neglecting electron transfer processes, is an over-generalization of a bonding model that refers specifically to the inorganic realm; whereas, based on Taber’s arguments, any ion pair interaction should be classified as ionic bond (e.g. ion pair interactions inside proteins).

From the educational side, we believe that students possess the conceptual tools needed for understanding ionic bonding. They are quite familiar with electrostatic phenomena at the macroscopic level, they know the meaning of charge attraction and repulsion. So, the diriment factor is the teaching practice. Teachers who promote discussion about the balance between attractive and repulsive forces between ions and the lack of directionality of electrostatic interactions may lead students to draw some logical consequences, i.e. the organization of ionic substances as crystal lattices and the lack of molecular entities.

In order to prevent the history conjecture, ionic bonding might be discussed in the frame of neutralization reactions followed by solvent evaporation, as a way to obtain ionic substances (Vladušić et al. 2016). In this case, ions are already found in the solution and there is no need to rely on electron transfer from neutral atoms. In doing so, attention is shifted to the interactions between ions instead of the process of ion formation. Interestingly, Vladušić et al. remarks that:

“Electron transfer reactions are the subject matter of the topic of oxidation-reduction processes, not of the topic of the structure of ionic substances” (Vladušić et al. 2016).

However, salts may also be obtained through redox processes and electron transfer justifies the existence of ions. A good compromise from the educational viewpoint is to focus, at first, on the macroscopic properties of ionic compounds, such as electric conductivity. In order to rationalise it, students may be invited to seek an explanation at the microscopic level. This leads to hypothesize the presence of ions, to reflect on the energetic of the process of salt formation and to deduce the presence of a crystal lattice and the impossibility for ionic molecules to exist, as a consequence of the non-directionality of Coulombic interactions.

An interesting issue to be discussed is the role of iconography and symbolic representations in conveying misconception on ionic bonding. Images like Figure 2.10 are problematic in several respect. They focus on single atoms (or ions), overshadowing the existence of a three-dimensional crystal lattice, so that students may take the NaCl formula as a molecular formula (in fact, NaCl and HCl are equivalent to an unaware reader). In addition, this representation of a reaction mechanisms may outshine the fact that it refers to millions of events occurring simultaneously at the microscopic level.

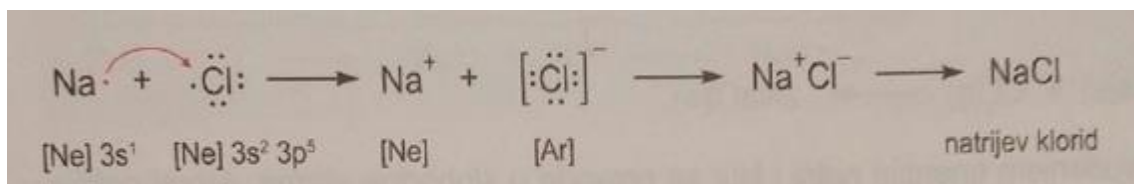


Figure 2.10 Description of ionic bond formation in a textbook (Vladušić et al. 2016)

To avoid feeding this kind of misconceptions, it helps focusing on the distinct macroscopic properties exhibited by ionic and molecular compounds. This comparison allows showing that ionic compounds cannot

be made up of neutral molecules. According to Bergqvist and Chang Rundgren (2017), in order to prevent students from "seeing" molecules everywhere, it is preferable to tackle chemical bonding by first discussing reticular substances.

Some recommendations aimed at preventing the onset of alternative conceptions on ionic bonding are (Vladušić et al. 2016):

- To avoid showing the formation of single ions;
- To remark that chemical formula indicates stoichiometric ratios and not microscopic structures;
- To remark that chemical formula of salts provide no information about the coordination number: in fact, it is challenging for students to cope with stoichiometric ratio and coordination numbers.
- To stress that ionic bonding results from the balance of attractions and repulsion forces involving the whole crystal lattice, and not just adjacent ions.

The previous suggestions are especially addressed to teachers who follow a traditional teaching approach to ionic bonding. We kept the above suggestions in mind while designing our teaching sequence, even though our choices are partly divergent from those proposed by authors like Taber and Vladušić.

We believe useful to introduce ionic bonding by looking at macroscopic experimental evidences that show that ionic compounds behave differently from molecular ones. The ionic bond model is introduced after the Lewis model. The need for a new bonding model arises from the evidence that the Lewis model cannot explain the properties of ionic substances. The mechanism of ion formation is presented in the classical way and justified by energetic reasons; then, specific activities are devoted to the notion of non-directionality which, in turn, leads students to develop the idea of a different structural organisation of ionic substances as compared to covalent ones.

Another source of alternative conceptions about chemical bonding comes from the so-called Octet Framework (Figure 2.11), discussed by Bergqvist (2016) and Taber (Taber and Coll, 2002). These scholars remarks that learning difficulties may arise from: i) lack of clarity on the driving force for bond formation; ii) anthropomorphic descriptions of chemical bonding; iii) insufficient focus on electrostatic forces involved in chemical bonding. The Octet framework originates from overrating the Octet rule and using it in a teleological way. This has many consequences in learners, especially as regards to covalent bonding. In fact, Taber and Coll (2002) remarks that "For many learners the shared electron pair *is the bond*, a notion which is somewhat lacking in explanatory power". So the main problem with the Octet framework is that the reasons why bonding occurs are not highlighted.

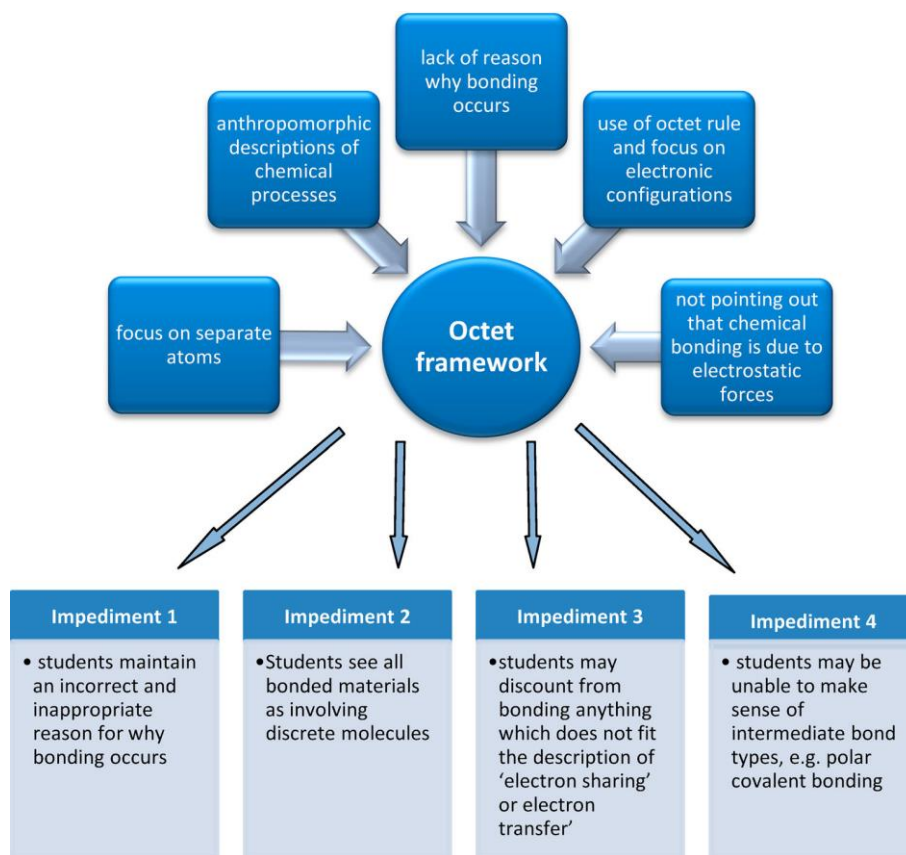


Figure 2.11 Description of the Octet framework (Bergqvist et al. 2016)

The use of analogies as a teaching expedient for building bridges between abstract concepts and everyday experiences is suggested by various authors (Ünal et al. 2006). Nevertheless, students' interpretation of analogies must always be verified, as it can be a source of alternative conceptions itself (Harrison and Treagust, 2000). For example, the use of stick-and-ball models may convey the idea that chemical bonds are sticks, i.e. physical objects (Coll and Taylor, 2001). Or, even worse, bonds' representations as sticks may lead students believe in the presence of covalent bonding in ionic or metallic lattices:

"A highly prevalent alternative conception for chemical bonding is that continuous covalent or ionic lattices contain molecular species suggest that *the ubiquitous use of ball-and-stick models used to model ionic lattices* may be instrumental in the generation of this alternative conception because students mistake sticks for individual chemical bonds" (Coll and Taylor 2001).

As we already mentioned, teachers must discuss communication codes with the classroom and accustom students to analyse iconography with a critical eye.

Incomprehension of the particle nature of matter and its representation are also diffuse and influence students' understanding of chemical bonding (Othman et al. 2008), Learning the particle nature of matter and the relationships between the molecular and macroscopic levels are necessary prerequisites: it is not possible to deal with atomic structure and bonding interactions (nucleo-electronic level) without a well-established knowledge of the particle model and its implications (Johnstone 2010; Bergqvist and Chang Rundgren 2017). So, a main source of alternative conceptions is rooted in the scarce epistemic awareness of teachers: whenever they do not discuss with the classroom the nature of models and their relationships with the physical realm, their rules and field of validity, their role of 'reasoning tools', they set the basis for the onset of severe alternative conceptions. Teachers rely heavily on textbooks for organizing their teaching contents: unfortunately, textbooks often do not tackle this subject sufficiently, even though it should be an introductory

content of any science course. In addition, too many textbooks adopt improper generalizations and oversimplifications in the description of chemical bonding. Or they omit relevant remarks:

“Only two teachers explicitly mentioned that all types of bonding are attractions between ‘positive and negative’ charges. These teachers taught using TB5, the only textbook that explicitly provided this description of attraction: ‘There are several different types of chemical bonding. But they are all the same thing, that is, attractions between positive and negative charges’ ” (Bergqvist and Chang Rundgren 2017).

Given the strong impact of initial and/or alternative conceptions on the learning process, many scholars recommend teachers to investigate them. Bergqvist et al. (2016) remarks that the common strategy of asking questions or answering students’ questions does not necessarily allow assessing students’ level of understanding. Effective diagnostic methods are written interviews through which students are asked to give written explanations and to draw structures or comments on drawings (Ünal et al. 2006). We applied this strategy for assessing students’ understanding of basic chemical notions, by getting relevant results (see the attachment 2). Multiple choice tests where students may choose between right and wrong options are also helpful, although answers may reflect alternative conception or random choices made by students. This is why multiple choice questions should always include the request to justify the choice made by students (Peterson et al. 1989; Taber 1997; Vladušić et al. 2016).

2.6 Lexical choices in the didactic transposition of the interatomic bonding

A final issue that needs to be mentioned is the role of lexical choices in science teaching and learning. Luigi Cerruti remarks the distance between natural and scientific language by saying that the latter is abstract and it is permeated by purely theoretical aspects (Cerruti 2020). The abstractness of chemical language plays a role in chemical education as it can hinder, along with other factors, the meaningful learning of concepts:

“The vast bulk of our teaching and learning is done through the medium of language. Language, lodged in long-term memory, takes part in the thinking processes in working memory and plays a major part in filtering incoming information. When language is particularly unfamiliar it takes up space in the working memory. Storage problems in long-term memory are created when a familiar word changes its meaning in another area of science, leading to misfiling and to the formation of alternative frameworks, the personal interpretations of what is heard or read ” (Johnstone 2010, italics added).

In order to find anchoring points in students’ memory, scientific terms have to relate with students previous knowledge and experience, otherwise they keep devoid of meaning and may foster the onset of alternative conceptions.

“Chemistry should be presented in a way that capitalizes on what students are familiar with and for which they already have anchorages in long-term memory. *This might require a complete reordering of what is taught*” (Johnstone 2010).

This is relevant in determining the teaching structure of a science course: macroscopic phenomena (which involves the use of a more familiar language) come first; microscopic and symbolic reasoning, i.e. the theoretical level (which implies a more abstract language) follow.

Taber and Coll remark:

“So it is important *to clearly signpost* the transitions, and make sure that we model the way chemists use molecular notions to explain macroscopic phenomena which have distinctly different features” (Taber and Coll 2002, italics added).

The transition is marked by a language shift. Whenever the two explanatory levels are mixed up (improper use of language), problems occur. For example, students may associate macroscopic properties of substances with microscopic particles: “We must be careful to ensure that *substances, and not molecules*, are said to evaporate, melt, expand, reflect, conduct and so forth” (Taber and Coll 2002, italics added).

As regards to lexical choices related with the notion of chemical bonding, Taber and Coll remark that:

“Bonding has a peculiar position in the molar-molecular scheme: for *we often talk of bonds as if they are macroscopic properties of materials*, so here we need to be particularly careful to ensure we are clear about the level of description we are employing” (Taber and Coll 2002).

Teachers need to pay special attention not to confuse molar and molecular levels, as this generates confusion in students’ thought. As regards to chemical bonding, it is debated whether the terms ‘bond’ and ‘interaction’ are equivalent or not. Several authors argue that using the term “interactions” as opposed to “bonds” promotes a dichotomous view of bonding, preventing students from grasping the relationship of continuity between inter-atomic interactions. In fact, Cooper et al. report:

“Some authors have recommended that *intermolecular forces such as hydrogen bonding or London dispersion forces be considered as bonds* and there is a compelling argument that bonds and intermolecular forces be considered part of a continuum of interactions between atoms” (Cooper et al. 2015).

The matter is delicate, as it is not just a terminological issue: it reflects a theoretical stance. Inter- and intra-molecular bonds not only differ in terms of formation mechanisms, bonding energy, directionality, etc. Behind this terminological choice lies the distinction between physical and chemical processes. Many textbooks state that inter-molecular bonds are broken in physical changes, whereas intra-molecular bonds are broken in chemical changes. So, this terminology might provide students with classification criteria. Nevertheless, many scholars remark the difficulty of students to deal with this terminology:

“These differences, while quite apparent to the expert, are clearly not so obvious to students. It is our contention that students who do not have a firm grasp on the forces that act both within and between molecules will be unable to make sense of phase changes, solution formations, and chemical reactions. *While experts may point out that the word “intermolecular” actually defines where the forces act*, it has been well documented, both in this study and in other reports, that *students have difficulty using terminology appropriately*” (Cooper et al. 2015, italics added).

The similarity of the two terms seems to be part of the problem:

“As might be expected students are readily confused about the differences between intermolecular and intramolecular forces in part at least *because of linguistic similarity of the terms*. Students often incorrectly identify intermolecular forces as the forces within a molecule or continuous covalent solid, and equate intermolecular forces with covalent bonds and are unaware of differences in strength of covalent bonds as compared with intermolecular forces” (Ünal et al. 2006, italics added).

Another problem is represented by anthropomorphic language, that is unanimously criticized by scholars:

“The evidence about using anthropomorphic and other metaphorical language to teach chemistry is more equivocal. *In the long term, we do not want our students to think that molecular interactions are like social interactions*, and can be explained in terms of psychological drives” (Taber and Coll 2002).

“In the common language of many chemistry students and instructors, *atoms and molecules are portrayed as very needy things*. They take or give away electrons because they “want” to fill their valence shells or satisfy the octet rule. [...] *For many chemistry educators, anthropomorphizing atoms and molecules and building explanations in terms of wants or needs (teleological explanations) are useful pedagogical strategies* for facilitating student understanding of abstract chemical models about the structure and properties of matter at the submicroscopic level” (Talanquer 2013).

This usefulness is clearly apparent, as it conveys alternative conceptions that will need to be eradicated. Taber and Coll remind the need to replace the familiar images created in the minds of students with scientific explanations that drastically avoid the use of humanizing expressions. clearly state this:

“The professional pedagogic skill of the teacher is needed to make sure that such comparisons become the anchors for more scientific descriptions and explanations. *Whenever anthropomorphic language is used it should be followed by subsequent reiterations in more formal scientific terms. If learners’ anthropomorphic comments are indulged in class, they could still be reflected back in more technical terms.* Learners can be challenged to translate their explanations into a form that does not call upon needs, wants, desires, preferences and what the atom might be thinking. In this way their ‘conceptual ecologies’ can be shifted to provide the fertile ground needed for the development of more scientific models of the chemical bond” (Taber and Coll 2002).

The previous examples show some controversies concerning the most appropriate terminological choices to be made in didactic transposition of chemical bonding. The didactic problems related to the use of language and specific terminology are innumerable. This synthetic paragraph cannot provide an exhaustive report of the literature on this issue. We just aimed at highlighting the relevance of linguistic aspects in the teaching practice of chemistry. Teachers are called to pay close attention and caution in the description of the phenomena, which is necessarily mediated by the language.

2.7 Conclusions

Figures 2.1, 2.2 and 2.3 summarize the main pieces of information available in the recent literature on chemical education as regards to the teaching of chemical bonding. Our survey highlights a number of issues pertaining both the conceptual/epistemological field and the educational/cognitive one. In summary:

- There is a need for new teaching strategies and devices aimed at overcoming students’ difficulties in learning chemical bonding and preventing the onset of alternative conceptions (Ünal et al. 2006). This thesis work is part of this research line;
- Several scholars remarks that educational research on chemical bonding needs to be further encouraged, in order to improve the teaching quality of this foundational chemical notion. Educational research outcomes may gradually lead to a revision of chemistry curricula at all school levels;
- Many theoretical suggestions are available in the literature as to how to improve the effectiveness of chemical bond teaching and avoid the spread of alternative concepts. These suggestions need to be turned into concrete teaching practices. This PhD work aims at providing a contribution in this regard;

- Our literature survey highlighted the scarce contribution of Italian scholars to educational chemical research. This reflects on the quality of the teaching practice of chemistry in Italian schools. A further critical element is that, in Italian schools, chemistry is often taught by teachers who have not been specifically trained in the chemical discipline and have limited knowledge of what ‘thinking chemically’ means. This often results in ineffective chemistry teaching practices and highlights the urgency to promote good practices of didactic transposition for chemistry.

Our literature survey on chemical bonding allowed us to highlight strengths and weaknesses of current educational practices on the issue of chemical bonding. Based on these results, we compiled a map of criteria which our teaching sequence will stick to:

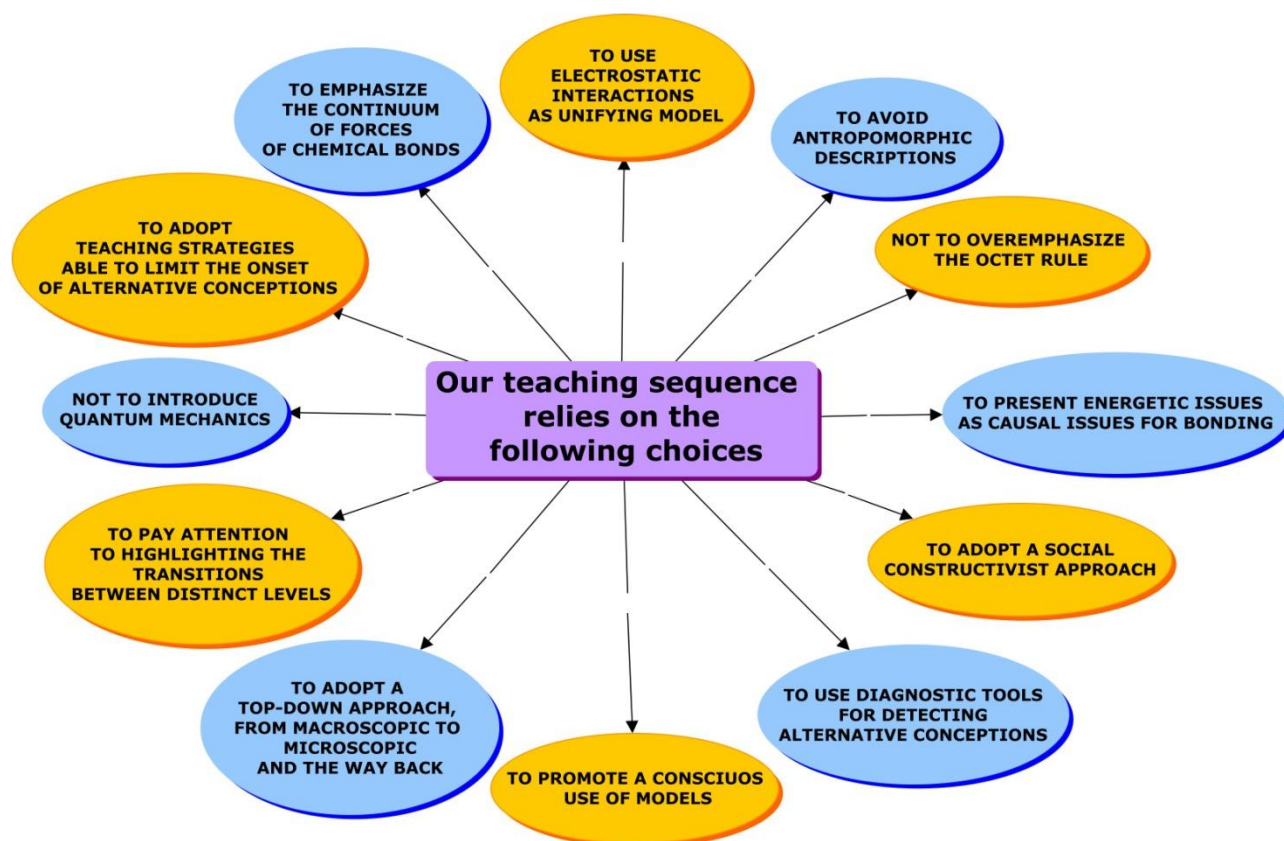


Figure 2.12 Summary of the choices made in designing the didactic sequence on chemical bonding which is presented in chapter

4

These choices will be duly discussed in chapter 4, that reports the analytical description of the sequence. Here, we wish to highlight only a few relevant aspects:

- The order according to which the different types of chemical bonding models are proposed, in the traditional approach, neither promote the idea of the common electrostatic basis of all kinds of inter-atomic interactions nor it highlights their relative energy scale. Traditionally both teachers and textbooks follow this order: ionic bond, pure covalent, polar covalent, metallic. Many scholars suggest a different order: pure covalent bond, polar covalent, ionic, metallic (Dhindsa and Treagust 2014) based on energetic arguments. We made the original choice of starting from weak intermolecular forces, in order to consider, at first, monoatomic substances displaying a single type of inter-atomic interactions.
- Our didactic choice of not relying on quantum mechanics and using, instead, the notion of electrostatic interaction as a central notion throughout the whole sequence is in agreement with the

position of many scholars. It is justified by the need to enable students to assign meanings to the proposed concepts and to propose models that are intelligible to them.

- iii) The choice to constantly emphasizing the common electrostatic origin of all types of bonds aims at avoiding the dichotomous conception of inter-atomic interactions, which is denounced as a problem by didactic research.
- iv) The choice to underline the energetic aspects and the relationship between energy and stability of the inter-atomic interactions has the purpose of underlining the aspects of continuity between the various types of interactions. A consequence of this approach is the avoidance of the teleological use of the octet rule.
- v) The choice of a socio-constructivist approach is a reaction to the proven ineffectiveness of transmissive teaching, which does not consider the importance of the learner's personal involvement in the learning process.
- vi) The choice to insist on the concept of model and its character of interpretive tool aims at clarifying the nature of scientific knowledge and training students at identifying perceptual facts and explanatory models. In all phases of the sequence, strategies are adopted to clearly differentiate the macroscopic evidence from the theoretical constructs that justify it.
- vii) The relationship between perceptual facts and explanatory models that characterizes scientific interpretation relates with the relationship between macroscopic and microscopic (atomic-molecular) aspects of reality, which is typical of chemistry. In sequence, great attention is paid to emphasizing the transitions between macroscopic, microscopic and symbolic levels.
- viii) The use of anthropomorphic descriptions (e.g. chemical bond as a “hug” between atoms) is denounced as a problem by many authors, as it favors the spread of alternative conceptions. Therefore we have carefully avoided its use in any context.
- ix) Given the impact that students' initial conceptions have on the entire learning process, we developed a specific questionnaire (see the attachment 2) to explore students' initial conceptions on some basic chemical topics, propedeutics to chemical bonding (e.g. particle model, the atomic structure, the concept of atom, molecule, simple and compound substances, mixtures, etc.).

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Chapter 3

Historical-epistemological evolution of the concept of interatomic bond

Introduction

Knowledge of the historical evolution and epistemological reflection on scientific concepts are crucial for science teaching. The historical-epistemological analysis of disciplinary contents allows deconstructing disciplinary contents in order to identify key-ideas and foundational concepts and to connect them together, in a network of associative connections. While developing didactic paths, teachers need to be aware of the conceptual knots inherent in the topics discussed with the classroom: the historical-epistemological analysis of teaching contents is precisely aimed at highlighting these knots. Therefore, knowledge of the epistemological foundations of its discipline should be part of the cultural and professional requisites of a good teacher.

Science, with its own methods, formulates laws, builds models, proposes theories, but these constitutive elements of scientific knowledge, once acquired, do not retain their validity indefinitely. They undergo continuous revisions over time. History of science is studded with conflicts between theories. It often occurs that the onset of new theories, more powerful or effective than previous ones, overcomes previous conceptions and fosters changes of paradigms, according to Kuhn's view (this is the case of Lavoisier's theory of combustion vs. the phlogiston theory). Therefore, scientific theories are historically situated products, conceived in a discovery context that undergoes continuous changes. Hence, science may be thought of as a progressive conquest of truth, a relative truth influenced by cultural and scientific contexts, without claims of being an absolute knowledge.

The historical dimension of science, intended as a cognitive process aiming at a relative truth, should be part of the teaching process. In this respect, the historical reconstruction of a discovery or a theory has a profound methodological, cultural and educational value.

Scientific progress is due to the discovery of new perceptual facts, to the invention of new conceptual tools, to the emergence of new concepts, but previously established knowledge is always in the background of these forms of internal discontinuity in the development of scientific knowledge. That's why studying history of science and the evolution of scientific ideas is crucial to understanding and interpreting scientific progress. This is true for any discipline and chemistry is no exception, especially when considering the role played by chemistry in science history:

“There is no doubt that chemistry plays an extremely relevant role in the history of science. Hence the primary need to cultivate and spread the history of chemistry. To introduce history of chemical culture into secondary school programs neither means bending to needs of sociology of science, nor means adopting a teaching practice where the role of theories and technical aspects of the discipline is forgotten. Obviously, chemistry has to be taught and students have to learn it. This is rather matter of making quality prevail over quantity, of making methodological aspects prevail over data acquisition, of devising problems rather than seeking technical solution. It's matter of highlighting the cultural values of this discipline” (Ciardi 2007, my translation).

This has relevant implications in the educational field. If science is conceived as a process wherein concepts and models are elaborated and made evolve, then meaningful learning approaches cannot neglect such evolution. This implies making precise didactic choices as regards to the level of modeling to be adopted at the various school levels, according to a conceptual sequence that is justified precisely by the historical evolution of concepts. As a result, it may turn inappropriate to discuss a topic by taking the most advanced

concepts and models (i.e. those very models used by scholars) as the starting point. Aim of a good teaching practice is understanding, i.e. a process that allows students to assigning meanings to what they learn. This requires going step by step, complying with conceptual propaedeuticities: first, simpler models are introduced in order to allow consolidating foundational concepts; these simpler models need to undergo evolution or to be replaced by new, more powerful models, This task can be accomplished by proposing increasingly complex problem-situations, whose design should reflect the historical and conceptual evolution. Despite the educational potential of studying the historical development of concepts, this aspect is often neglected in science (and chemistry) teaching:

“According to many authors, the introduction of the history of science into school curricula and university teaching is a recent phenomenon, and yet remains very fragmentary, and spread unevenly between various school levels and different types of schools. In fact, a careful analysis of school textbooks reveals either the absence of historiographic approaches to chemical education or the uneven presence of science (and chemistry) history as marginal items in the didactic path, completely detached from the discussion of those foundational concepts that students should learn and master during their school career” (Carlone et al. 2018, my translation).

Yet, the historic-epistemological approach has greater chance to lead students towards meaningful learning and minimize the onset of alternative conceptions as compared to other approaches (Croft and de Berg 2014). This applies to many foundational chemical notions, namely the concept of chemical bonding. According to the traditional teaching approach, *a priori* classification of substances according to the categories defined by various bonding models (ionic, metallic, covalent and reticular substances) is generally proposed as the starting point. By doing so, any reference to the phenomenology that calls for these explanatory models goes lost. The conceptual knots that have punctuated the historical path that led to designing all different bonding models lay unexploited from the teaching viewpoint. As a consequence, students risk to confuse phenomena with their models; the need for distinct models as explanatory tools for distinct phenomenologies is overshadowed. Such multiplicity becomes an undemonstrated fact, instead of expressing specific explanatory needs, arising from the multiple behaviors of substances found in nature. In other words, the relationship between observation and interpretation is never clarified. The scientific logic is overturned, as the illustration of the explanatory models actually precedes the questions that (historically) generated them. Another disadvantage of the traditional approach to chemical bonding is the lack of clarification of the nature and function of classifications⁹: a rigid classification of the types of substances and chemical interactions, proposed before introducing the bonding models they refer to, is counterproductive as it eludes the problems inherent in any type of classification and does not allow grasping aspects that are transversal to the classification classes. For example, the phenomena classified under the different classes of interatomic interactions are perceived as unrelated to each other, their common physical basis is not understood by students, who finally do not catch the continuity of bonding forces (Levy Nahum et al. 2008).

The historical-epistemological approach to chemical bonding allows highlighting the conceptual knots typical of this topic; in doing so, it may suggest operational choices that limit the onset of the most common alternative conceptions, by taking into account both pedagogical and didactic aspects. As meaningful learning is achieved whenever significant points of connection are established between students' mental structures and the

⁹ Classifications in science play a fundamental role and are widely used by all disciplines; despite the foundational character of classifications in disciplinary knowledge, their meaning and role is never clarified to students, who consequently take them as factual data, instead of theoretical constructs functional to the cognitive purposes of each discipline (Soavi et al., 2012).

conceptual structure of the knowledge to be learned (Roletto 2005), then it is not advisable to propose theories, concepts and models that require cognitive tools not yet available to students. Hence, at high school level, chemical bonding models need to rely on notions whose meaning is accessible to students; this is the case of the Lewis model and the law of electrostatics applied to the microscopic realm, that are the notions that chemists used to apply before the advent of quantum era. It is crucial to understand that, despite their being outdated from the technical viewpoint (because they are based on the description of the electron as a particle and lack the explanatory and predictive power of more recent and technically updated models), these models maintain a didactic value that should not be underestimated, as they are tools which allow students to assign meaning to the notion of chemical bond and to understand its role in chemistry. It is precisely the history of concepts that suggest the impropriety of presenting advanced quantum mechanics models (that describe the electron as a wave, introduce the concepts of orbital, probability density, and finally describe bonding as a wave interference) to school students. The explanatory power of the most recent models is undoubtedly wider as compared to previous ones: in fact, they are used by experts and are discussed in university educational contexts, when they are combined with a suitable wealth of mathematical and physical knowledge. Nevertheless, even at the university level, old models are not completely abandoned and still play a heuristic role: just think of how organic chemistry and biochemistry still use Lewis structures or the Lewis model to schematize the migration of electron doublets in organic synthesis, where the electron is thought of as a particle, not as a wave). Finally, it is worth stressing that the very same university students who are exposed to the most advanced descriptions of chemical bonding still rely on mental images that comes from previous bonding models: would they be able to provide the utterly abstract quantum mechanical descriptions with a meaning without having previously been exposed to more intuitive models, such as the Lewis model?

Therefore, it is worthwhile to retrace the history of the concept of chemical bonding and other related notions, to focus on the logical and epistemological relationships between them, and to reflect on the conceptual obstacles that chemists had to face in developing the bonding notion.

3.1 Historical-epistemological evolution of the concept of interatomic bonding

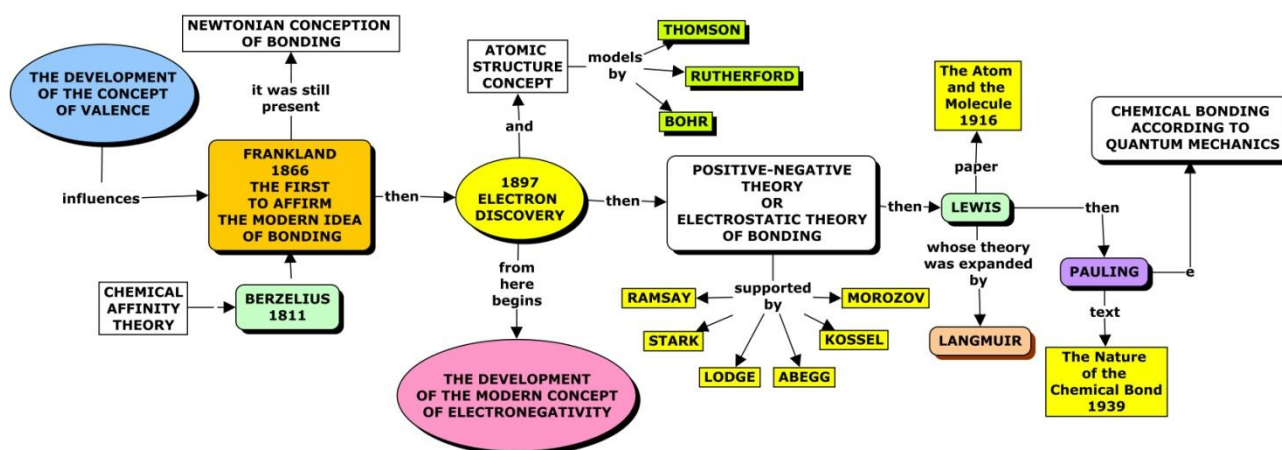


Figure 3.1: Summary map of the historical development of the idea of chemical bonding and related concepts

The attempts to explain how atoms join together dates back very far in history, but Edward Frankland (1825-1899) was the first to use the term ‘bond’ in a 1866 paper published in *J. Chem Soc.*:

“By the term *bond*, I intend merely to give a more concrete expression to what has received various names from different chemists, such as *an atomicity*, *an atomic power*, and *an equivalence*. A

monad is represented as an element having one bond, a dyad as an element having two bonds, etc. It is scarcely necessary to remark by this term *I do not intend to convey the idea of any material connection between the elements of a compound*, the bonds actually holding the atoms of a chemical compound being, as regards their nature much more like those which connect the members of our solar system” (cited in Sutcliffe 1996, italics added).

In this quote, Frankland underlines the *immaterial* nature of chemical bonds by using the concept of remote interaction, borrowed from classical physics. Frankland's idea of comparing chemical bonding to gravitational interactions between planets clearly derives from Newton's theories (1643-1727). The Newtonian interpretation of chemical bonding as a gravitational attraction between atoms survived for a long time, despite its several limitations. In fact, unlike planetary systems, atomic systems were experimentally inaccessible: how to measure interatomic distances, atomic radius and masses? Furthermore, the selectivity of chemical bonding could not be justified by Newton's explanation, since masses were not the factor responsible for bonding. Finally, a gravitational model would imply a net of interatomic interactions linking all atoms in the molecule, which clearly cannot be the case (Villani 2001 p.83).

3.1.1 The notion of valence

In 1866, Frankland came to conceive the idea of bonding through the development of the valence notion. He established that atoms possessed the ability to saturate their valences with a number of atoms from another element:

“When the formulae of inorganic chemical compounds are considered, even a superficial observer is impressed with the general symmetry of their construction. The compounds of nitrogen, phosphorus, antimony and arsenic especially exhibit the tendency of these elements to form compounds containing 3 to 5 equivs. Of other elements, and *it is in these proportions that their affinities are best satisfied*; thus in the ternary group we have NO₃, NH₃, NI₃, NS₃, PO₃, PH₃, PCl₃, SbO₃, SbH₃, SbCl₃, AsO₃, AsH₃, AsCl₃,....; and in the five-atom group, NO₅, NH₄O, NH₄I, PO₅, PH₄I, ... Without offering any hypothesis regarding the cause of this symmetrical grouping of atoms, it is sufficiently evident, from the examples just given, that such a tendency or law prevails, and that, no matter what the character of the uniting atoms may be, *the combining-power of the attracting element, if I may be allowed the term, is always satisfied by the same number of these atoms*” (Frankland 1852, italics added).

The combining-power of the attracting element is the combinatorial potential of atoms, which according to Frankland, is characterized by a certain symmetry and recursiveness: in the absence of a clear explanatory hypotheses, Frankland remarks that this reflects some intrinsic property of atoms. The concept of valence had further developments and implications, always intertwined with the evolution of the concept of chemical bonding. However, the notion of valence aimed at highlighting a quantitative selectivity of atoms, rather than offering a causal explanation (Villani 2001, p. 84). The problem of the combinatorial potential of atoms was discussed throughout the 19th century. J.J. Berzelius (1779-1848) remarked that the (still undemonstrated) hypothesis that bodies were made by indivisible atoms did not, in itself, imply atomic combination according to constant proportions for each kind of atom. Clearly, more should have been known about how atoms bind together (Villani 2001 p. 86). In fact, based on the sole law of multiple proportions, the combination of indeterminate quantities of two different kinds of atom could result in countless compounds, characterized by distinct combinations, hardly separable from each other. With these considerations, Berzelius raised the problem of the combinatorial capacity of atoms, that is, of valence.

In 1821 Amedeo Avogadro (1776-1856) came to the conclusion that two halogen atoms always combined with one oxygen atom and, similarly, one oxygen atom was saturated by one sulfur atom. Based on substitution theory, A. Laurent (1807-1853) and J.B. Dumas (1800-1884) proposed the quantitative equivalence of chlorine and hydrogen. These results led C.F. Gerhardt (1816-1856) to develop his theory of types and to state the rule (1846), according to which the number of carbon and oxygen atoms in organic compounds can be odd or even, whereas the number of hydrogen atoms is always even (Solov'Ev 1976 p. 210). In modern words, we would say that the sum of the atoms with odd valence is always an even number (e.g., the number of hydrogen atoms in hydrocarbons is even) (Solov'Ev 1976 p. 210). These experimentally observed regularities allowed Gerhardt and Laurent to draw conclusions on the number of atoms in molecules and to correct mistake made in chemical analysis and the formulas. From 1850 on, the notion of valence began to be outlined. Carbon atoms were shown to bear 4 hydrogen atoms or two oxygen atoms at the utmost. The saturation potential was shown to be one for H, Li, K, Na, Cl, Br, or two for Zn, Ca and Ba. It is precisely the ability of atoms to saturate with a certain number of atoms of another element that led to the concept of valence. In 1852 E. Frankland and B.C. Brodie (1817-1880) developed the idea that single atoms exhibit specific saturation power in compounds. In 1851 W. Odling first introduced inverted comma in the symbols of elements to indicate their valence: H ‘, K’, Cl ‘, O’ ‘etc. In his 1858 article “*Über die Constitution und die Metamorphosen der chemischen Verbindungen und über die chemischen Natur des Kohlenstoffs*”, F.A. Kekulé (1829-1896) meticulously justified the tetravalence of carbon and clarified the meaning of the general formula of saturated hydrocarbons (C_nH_{2n+2}), already deduced by Gerhardt. Kekulé also highlighted the fundamental idea of the ability of carbon atoms to bind together and form long chains, an idea that played a decisive role in the advancement of organic chemistry. Unlike Kekulé, A.S. Couper (1831-1892) acknowledged that elements' quantitative affinity, that is valence, could be variable. For example, the valence of nitrogen can be 3 or 5. According to Couper, carbon was characterized by “two degrees of affinity” towards oxygen, a lower one, as in carbon monoxide (CO), and a higher one, as in carbon dioxide (CO₂). Moreover, constant valence would not justify the structural formula of many inorganic compounds, such as ammonium chloride NH₄Cl, phosphorus pentachloride PCl₅ and others. In fact, in organic chemistry, carbon is always tetravalent, hydrogen is monovalent and oxygen is divalent: this supports the idea of constant valence. Conversely, in inorganic compounds, nitrogen, sulfur, phosphorus and other elements show various valences. These behaviours highlighted that valence is not an intrinsic property of isolated atoms, but a relational property, as it depends on two factors: the nature of bound atoms and the reaction environment.

3.1.2 The notion of chemical affinity

Back to the concept of chemical bonding, what Frankland designates as *bond* is rooted in the notion of *chemical affinity*, familiar to the early 19th century chemists. Chemical affinity was meant as "the tendency of one body to combine with another" according to Claude-Louis Berthollet (1748-1822) (Zingales 2005). The idea that bodies similar in nature may exhibit a reciprocal affinity dates back to antiquity and derives from an old alchemical principle which is still sometimes used today, albeit in different forms and contexts: "Similar attracts and joins its similar". The French chemist and physician Geoffroy (1672-1731) was the first to build an affinity table. Jean Philippe de Limbourg (1726-1811) and Torbern Bergman (1735-1784) later published other more complete affinity tables. Although all of these "Affinity Tables" had imperfections (they were qualitative tables), nevertheless they had been useful tools for predicting whether a chemical transformation might take place or not. Bergman, in a work dated 1775, defined ‘chemical affinity’ as an attraction that reflects the tendency to combine according to the logic that the strongest prevails. In fact, he argued that “Substance C replaces substance B within compound AB, resulting in compound AC, due to its greater attraction with substance A” (Fichera 2015). The French chemist Pierre Joseph Macquer (1718-1784)

attributed great importance to the concept of chemical affinity. In chapter II of his first work (*“Eléments de chimie théorique”*, published in 1749) titled *“Idée générale des rapports des différentes substances”*, Macquer listed seven rules relating to chemical affinity. In summary, he stated that, if one substance shows affinity for another substance, they join together and form a compound; similar substances are affines. After joining together, substances lose some of their former properties; in addition, they can recombine, based on their relative affinity (Fichera 2015). About 30 years later, in 1782, another French chemist, Antoine François Fourcroy (1755-1809), published the work titled *“Eléments d'Histoire Naturelle et de Chimie”* where he stated a new idea: chemical affinity is displayed by substances of a different nature, whose combination result in new, original substances, whose properties may differ from its parent substances. His interpretation was effective in giving account of macroscopic phenomena and was quickly accepted by the scientific community (Jensen 1996).

3.1.3 The electric properties of matter, Berzelius’ dualistic theory and the origin of the electronegativity notion

Contextually to the evolution of the notion of chemical affinity, in 1800 Alessandro Volta (1774-1827) described for the first time a simple machine capable of producing electrical current, i.e. a battery. His work concurred to highlight the links between electricity and chemical transformations: they stimulated scientists' reflections on the nature of bonds within chemical compounds (Fichera 2015). It is from these experiments that the view of chemical bonding as an electrical phenomenon started to develop, although the discovery of the electron (1897) was still far away.

Electrochemische Theorie.	
Sauerstoff,	Palladium,
Schwefel,	Quecksilber,
Stickstoff,	Silber,
Fluor,	Kupfer,
Chlor,	Uran,
Brom,	Wismuth,
Jod,	Zinn,
Selen,	Blei,
Phosphor,	Cadmium,
Arsenik,	Kobalt,
Chrom,	Nickel,
Vanadium,	Eisen,
Molybdän,	Zink,
Wolfram,	Mangan,
Bor,	Cerium,
Kohlenstoff,	Thorium,
Antimon,	Zirkonium,
Tellur,	Aluminium,
Tantal,	Yttrium,
Titan,	Beryllium,
Kiesel,	Magnesium,
Wasserstoff.	Calcium,
	Strontium,
Gold,	Barium,
Osmium,	Lithium,
Iridium,	Natrium,
Platin,	Kalium.
Rhodium,	

Figure 3.2: Berzelius’ electronegativity table of 1836. The most electronegative element (Oxygen or Sauerstoff) is listed at the top left and the least electronegative element (Potassium or Kalium) is listed at the lower right. The line between hydrogen (Wasserstoff) and gold separates predominantly electronegative elements from predominantly electropositive elements (Jensen 1996).

The chemists who were mostly engaged in studying electrical phenomena were Davy (1778-1829), Faraday (1791-1867) and Berzelius (1779-1848), the father of the first electrical theory of chemistry. Between 1811 and 1818 J.J. Berzelius widely used electrochemical concepts to develop his own theory of chemical affinity (Sutcliffe 1996; Stranges 1984; Jensen 1996). Berzelius described chemical affinity as the result of electrical attractions between *electropositive* substances (which in electric batteries concentrated at the negative pole) and *electronegative* substances (that collected around the positive pole of the battery). He later designed a table (Figure 3.2) where he ordered the known elements in a series starting with oxygen (the most electronegative element of all) and sulfur and ending with the alkali and alkaline earth metals (Mg, Ca, Sr, Ba, Na, K). Potassium was the last one because it was considered as the most electropositive. The greater the distance between the elements in the table, the greater the chemical affinity and stability of the resulting compound, as distant elements exhibited very different *polar intensities*. The term *polar intensity* comes from Berzelius's hypothesis that electricity was distributed in different proportions inside atoms, depending on the type of element. According to this conception, the negative portion clearly prevails over the positive, in oxygen; this explain why oxygen develops at the positive pole during electrolysis. Potassium displays a specular behavior: in fact, it is collected at the negative pole. Hence, the *dualistic* character of Berzelius' theory. He also pointed out that the electrical character of an element is relative, since it depends on the atom with which it is compared (Figure 3.3): in this perspective, sulfur can be electronegative with respect to a metal, but electropositive with respect to oxygen (Fichera 2015; Villani 2001 p. 86). This last remark is especially interesting because it anticipates to some extent the modern concept of electronegativity.

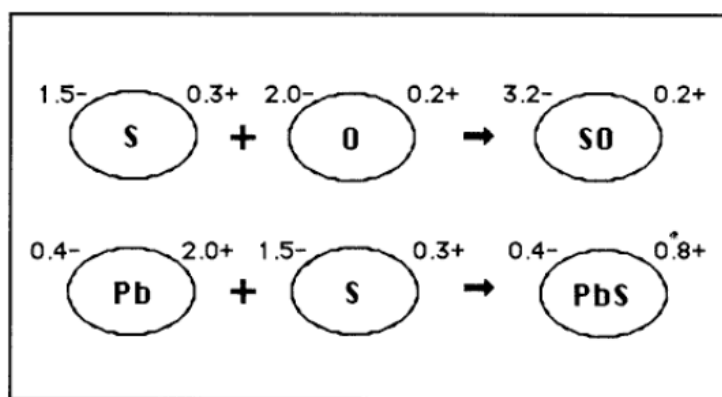


Figure 3.3 Top: A modern visualization of Berzelius model for the reaction between two predominantly electronegative atoms leading to enhancement of the electronegative unipolarity of the product and to the formation of an acid compound. Bottom: A modern visualization of Berzelius model for the reaction between a predominantly electronegative atom and a predominantly electropositive atom leading to a decrease in the unipolarity of the product and to the formation of a relatively neutral compound. Fractional charges have been used in order to suggest a fluid model of electricity rather than a particulate model (Jensen 1996).

Interestingly, Berzelius' scale matches quite well with Pauling's scale of electronegativity: the main discrepancy is for Pb. Berzelius' scale of 'electronegativity' meant to replace the *oxygenicity scale* proposed by the Italian physicist A. Avogadro (1776-1856). Avogadro followed Lavoisier's theory of oxygen as the principle of acidity; he attempted to build a scale of substance affinities based on the analogy between neutralization reactions between acids and bases (on one hand) and attraction between opposite charges (on the other) (Fichera 2015). Already in 1809, Avogadro emphasized the relative character of the concepts of acidity and basicity, foreseeing the possibility of generalizing them and applying them to chemical interactions, (Jensen 1996). He stated that: "If a substance A combines with a substance B, it is because one plays the role of acid and the other the role of base" (Avogadro 1809).

To implement this idea, Avogadro developed an oxygenity scale that allowed simple substances to be classified based on their tendency to react with other substances, taking oxygen as a reference element. The term *oxygenicity* used by Avogadro (to designate the property by which a body displays acid antagonism with

respect to a certain number of other bodies) actually meant what we will now call the *acidity scale*: oxygen in fact was at the top of the scale and acidity increased from metals to oxygen (Fichera 2015). The greater the separation distance of two substances in the oxygenity scale, the greater their chemical affinity (Figure 3.4).

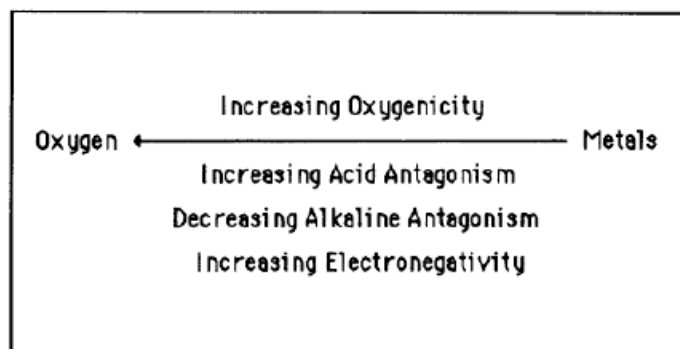


Figure 3.4: A modern visualization of Avogadro's oxygenicity scale and its correlation with both the relative acidity and alkalinity of substances and with their degree of electrical heterogeneity (Jensen 1996).

The discovery of hydracids undermined Lavoisier's theory of oxygen as the principle of acidity; this theory was superseded and Avogadro's proposal was left undeveloped (Fichera 2015).

Over time, Berzelius's electrochemical theory and his dualistic classification system were abandoned. However, the electronegativity notion remained and was developed in relation to chemical bonding.

3.1.4 Beyond Berzelius, new perspectives on chemical bonding

Although in the early 1800s the theories that supported the electrical attraction between atoms were dominant, many chemists cannot see electrochemical theories as a viable way to investigate the problem of interatomic interactions. This occurred for two main reasons: i) the lack of suitable experimental tools for quantitative measures of the electricity found in substances; ii) the progress made by organic chemistry research.

In fact, organic chemistry highlighted the weaknesses of Berzelius's electrical theory, as organic compounds are made of carbon atoms bound together, an evidence that Berzelius's theory could not justify (Stranges 1984). In addition, the variety of behavior of different substances called for multiple explanatory schemes for the still mysterious phenomenon of chemical bonding. It was precisely the investigation of the properties of saline solutions and organic compounds that, later on, after the discovery of the electron, would lead to the elaboration of a multiplicity of bonding models. In particular, the problem of the bonding mechanism between atoms of the same type would find satisfactory answers and adequate explanatory schemes only with Lewis and, even later, by quantum mechanics.

The relationship between electrical phenomena and chemical bonding became evident thanks to the contributions by many nineteenth century chemists. Among these, Svante Arrhenius (1859-1927) whose investigations on electrolyte solutions led to the formulation of the ionic theory (Arrhenius 1887, cited in Stranges 1984). Arrhenius formulated the concept of *electrically active molecules*. By this term, he designated what we now call electrolytes. In his Nobel lecture, in 1903, he underlined that only electrically active molecules are chemically active. Arrhenius associated chemical and electrical activity to the same cause, the presence of ions:

“I was thus led to the assumption that the *electrically active* molecules are also *chemically active*, and that conversely the electrically inactive molecules are also chemically inactive, relatively speaking at least.” (Arrhenius 1903).

However, the clarification of the nature of chemical bonding and the identification of electrically charged species involved in it was still to come.

A crucial step in the formulation of a coherent bonding theory was the discovery of electron, which occurred in 1897 thanks by J.J. Thomson (1856-1940). From this moment on, the concept of *atomic structure* was also been developed through the formulation of various models, usually discussed in chemistry texts. This conceptual step highlights a prerequisite still valid today: it is not possible to tackle the problem of chemical bonding from a modeling viewpoint without dealing first with atomic structure. From the educational viewpoint, this implies addressing atomic structure at a level that allows introducing those conceptual elements (electron, nucleus, nuclear charge, electronic shells) that are essential for understanding chemical bonding at a basic level.

J.J. Thomson, thanks to his studies on rarefied gases, was the first to establish that electrons were components of atoms. This important event paved the way for a univocal definition of electronegativity, a notion previously introduced by Berzelius. After his contribution, other scholars took up this notion and made it evolve during the second half of nineteenth century, with the aim of clarifying the notions of chemical bonding, valence and chemical structure. Then, with the development of the Periodic Table, electronegativity would have been identified as a periodic property. Before the discovery of the electron in 1881, Hermann Helmholtz hypothesized that neutral species contained equal numbers of positive and negative mobile charges; the ability of atoms to ionize related to their tendency to loose or gain charges. Within this model, the electronegative and electropositive character of atoms became a measure of inherent differences in atoms' ability to attract and hold electrical particles with opposite charges. The discovery of electron confirmed the presence of the negative charges suggested by Helmholtz. Furthermore, it suggested that a corresponding mobile "positive electron" would also been found soon. These hypotheses were supported by Walter Nernst. Other scientists rather sought for a unitary theory of electricity, according to which mobile negative particles could be added or removed from neutral atoms, their positive countercharge being an integral part of atomic nucleus. In the frame of this model, ionization was due to loss or gain of negative electrons, and electronegativity became a measure of this ability. A German physicist, Johannes Stark (1874-1957) was a strong supporter of this thesis. He described the tendency of chemical elements to become saturated with negative electrons, a tendency that depended on the values of the ionization energy:

“In a certain sense we have been describing *the tendency of the chemical elements to become saturated with respect to negative electrons*. And this saturation tendency differs from element to element in keeping with the magnitude of its ionization energy. The greater the force with which a chemical atom holds on to its own electrons, the greater its ionization energy, and in general the greater its saturation tendency for additional negative electrons. By way of example, the ionization energy, as well as the saturation capacity, of a chlorine atom is greater than that of a sodium atom (Stark 1903 cited in Jensen 2003).

Although many physicists and chemists believed that these two models of electricity were essentially equivalent, others argued that the unitary model was simpler and in better agreement with experimental evidence. The English chemist Geoffrey Martin was among the supporters of this model: in 1905, he stated that atoms can be electronegative or electropositive depending on the force with which electrons are held within atoms. Hence, according to Martin, atomic valence related with one type of electron. A unitary interpretation of electronegativity was being established; in 1913 Kasimir Fajans (1887-1975) argued that the electronegative character of atoms depends on their ability to lose or gain negative electrons:

“Electronegative character is defined as the inclination of an atom to split off or take on negative electrons” (Fajans 1913 cited in Jensen 2003).

Furthermore, chemists also began to correlate this character with atomic size: according to Norman Campbell (1907), smaller atoms hold electrons more tightly than larger ones. Interestingly, when Linus Pauling (1901-1994) proposed a quantitative formulation of electronegativity of the elements, in 1932, he did not provide a qualitative definition for this concept. He clearly assumed that his readers were familiar with it, since this notion had been part of chemical thinking for more than a century and its most recent definition, in terms of an atom's ability to attract valence electrons, was almost 30 years-old. Surprisingly, the 1960 edition of "The Nature of the Chemical Bond" by Pauling reports a qualitative formulation of electronegativity: Pauling states that *electronegativity* represents "the power of an atom in a molecule to attract electrons to itself" or even "the attraction of a neutral atom in a stable molecule for electrons" (Pauling 1960 pp. 88 and 95). The correlation between electronegativity and heat of reaction is discussed by Pauling in 1932 and exposed in his article titled "The Energies of Single Bonds and the Relative Electronegativities of Atoms" (Pauling 1932). In the same period, the correlation between electronegativity, ionization energy and electron affinity (or atomic tendency to electron saturation) discussed by Stark, Martin and Fajans, [was](#) examined by Robert Mulliken in his 1934 paper "A New Electroaffinity Scale":

"A new approximate "absolute" scale of electronegativity, or electroaffinity, is set up. The absolute electroaffinity on this scale is equal to the average of ionization potential and electron affinity. These quantities must, however, in general, be calculated not in the ordinary way, but for suitable "valence states" of the positive and negative ion [...] The present electronegativity scale (like the others) is rather largely empirical, especially as to its quantitative validity [...] Nevertheless, the new scale has a degree of theoretical background and foundation which *throws some new light on the physical meaning of the concept of electronegativity*" (Mulliken 1934).

The quantitative definition of electronegativity proposed by Mulliken is simpler and more understandable as compared to Pauling's, because it is based on two measurable physical quantities, ionization potential and electron affinity. It's worth noting that electronegativity is formally defined: there is no final definition. Mulliken remarks that his definition has the advantage of making the physical meaning of electronegativity more understandable (Mulliken 1934). This remarks is valuable, from the educational viewpoint, as it underlines the need for a notion to be understandable by those who use it. Hence, in didactic contexts, Mulliken's electronegativity is preferable to Pauling's.

It is worth reminding that two other relevant attempts to provide a quantitative definition of electronegativity (Jensen 2012) were made by Worth H. Rodebush (1887-1959) and Groves H. Cartledge (1891-1980), well before Pauling. Rodebush was the first ever to propose an electronegativity scale, calculated as the V/S ratio, with V = number of valence electrons and S = number of shells:

"If it might be permissible to introduce a qualitative formula into science which is rapidly becoming exact, we might represent electronegativity as a function of V/S where V is the number of valence electrons and S the number of shells. *The basis of this formula is Coulomb's law* and I believe that in a few years we shall calculate the energy changes in chemical reactions by means of it" (Rodebush 1925 cited in Jensen 2012).

The electronegativity values calculated according to Rodebush (Figure 3.5) are very close to those of Pauling's. Hence, had Rodebush developed his idea thoroughly, electronegativity values for the elements of the main block would have been available already in 1925 (i.e. seven years before Pauling's article) (Jensen 2012). Furthermore, unlike Pauling's, Rodebush's definition of electronegativity was of the primary type, as it correlates atomic properties and had a clear theoretical justification, Pauling's definition was of the secondary type because it is based on empirical relationships between macroscopic data (bonding energies

from thermochemical measurements) and electronegativity. Finally, it is interesting to note that Rodebush scale unequivocally reflects the classifications of elements into metals and non-metals (Jensen 2012).

	1	2	3	4	5	6	7	8
2	Li (0.50)	Be (1.00)	B (1.50)	C (2.00)	N (2.50)	O (3.00)	F (3.50)	Ne (4.00)
3	Na (0.33)	Mg (0.67)	Al (1.00)	Si (1.33)	P (1.67)	S (2.00)	Cl (2.33)	Ar (2.67)
4	K (0.25)	Ca (0.50)	Ga (0.75)	Ge (1.00)	As (1.25)	Se (1.50)	Br (1.75)	Kr (2.00)
5	Rb (0.20)	Sr (0.40)	In (0.60)	Sn (0.80)	Sb (1.00)	Te (1.20)	I (1.40)	Xe (1.60)
6	Cs (0.17)	Ba (0.33)	Tl (0.50)	Pb (0.67)	Bi (0.83)	Po (1.00)	At (1.17)	Rn (1.33)
7	Fr (0.14)	Ra (0.29)						

Figure 3.5: The electronegativity values calculated with the Rodebush formula (Jensen 2012)

The electronegativity scale proposed by Groves H. Cartledge anticipated Pauling's by only by 4 years, as it was developed in 1928. Cartledge proposed a way of calculating the polarizability of cations or *ionic potential*: Z/r with Z net charge of the cation and r its radius. Jensen (2012) remarks that, as most cations correspond to atomic cores, the polarizability measures made by Cartledge are a measure of atom's ability to attract electrons, ie., electronegativity. Later on, Cartledge noticed that the square root of those values was a more suitable parameter, and he built his scale (Figure 3.6) which differs very little from Pauling's.

	1	2	3	4	5	6	7	8
2	Li (1.29)	Be (2.54)	B (3.87)	C (5.16)	N (6.71)	O (8.19)	F (10.0)	Ne (NG)
3	Na (1.02)	Mg (1.76)	Al (2.45)	Si (3.13)	P (3.83)	S (4.55)	Cl (5.20)	Ar (NG)
4	K (0.87)	Ca (1.42)	Ga (2.20)	Ge (2.74)	As (3.26)	Se (3.78)	Br (4.24)	Kr (NG)
5	Rb (0.82)	Sr (1.33)	In (1.92)	Sn (2.36)	Sb (2.84)	Te (3.27)	I (3.74)	Xe (NG)
6	Cs (0.77)	Ba (1.21)	Tl (1.78)	Pb (2.18)	Bi (2.60)	Po (3.02)	At (NG)	Rn (NG)
7	Fr (NG)	Ra (1.24)						

Figure 3.6: The electronegativity values calculated with the Cartledge formula (Jensen 2012)

Although both Rodebush' and Cartledge's scales provided quantitative values for electronegativity, they did not have the same impact and popularity as Pauling's. We end this digression on electronegativity and go back to issues related with the investigations of atomic structure, after the discovery of electrons.

3.1.5 Atomic structure models

The scientific problems that stimulated the formulation of various atomic models are summarized by the following questions: how were positive and negative charges distributed in the atom? How many electrons were present in atoms of different elements? How to justify atomic mass? The events that led to the formulation of the atomic models of J.J. Thomson, W. Rutherford (1871-1937) and N. Bohr (1885-1962) are renowned. Each model attempted improving the previous one, trying to explain experimental evidence that could not be justified by previous models, and improving those aspects of previous models that led to fallacious predictions of experimental results. For example, Rutherford proposed that the positive charge was concentrated in a small volume, the atomic nucleus, almost entirely responsible for the atomic mass. Whereas the Thomson model known as *plum pudding* was characterized by a uniform distribution of positive charges in space (with negative charges following concentric orbits in a plane), the Rutherford model was rather

characterized by vacuum and charge distribution asymmetry (with positive charges concentrated in the nucleus, and negative charges distributed all over, around the nucleus). Bohr's model aimed at justifying the stability of a system made of separate positive and negative charges, which clearly do not collapse into each other despite electrostatic attraction. Bohr formulated the hypothesis that electrons occupy orbits characterized by specific and fixed energy values. Later on, the birth of the new wave theory of matter, which describes electrons as waves, led to the formulation of atomic quantum model (1926) characterized by the notions of orbital (that replaces the classical orbit notion) and wave function, thus marking the transition from a deterministic to a probabilistic description of the physical realm (Schrödinger 1887-1961). The problem of the discrepancy between the atomic mass values and the sum of protons and electrons masses was still to be solved. In 1932 James Chadwick (1891-1974) discovered the neutron, a particle as massive as proton, but electrically neutral. The neutron provided an explanation for the existence of isotopes, discovered by Frederick Soddy (1877-1956) just over a decade earlier. Therefore, in less than twenty years, two main features of classic atomic theory fade away, i.e. the elementary nature of atoms (as atoms turned out to be structured particles, made of sub-atomic components) and the homogeneous nature of elements (as atoms of a same element turned out to form an isotopic mixture) (Villani 2001 p. 99; Ghibaudi et al. 2020 p. 265).

3.1.6 Electrical theory of bonding

Back to the evolution of the concept of chemical bonding, a crucial question was now to understand the relationship between electrons and the electrical forces responsible for interatomic bonding. The tiny mass of electrons as compared to nuclear mass clearly suggested the great mobility of electrons with respect to the atomic nucleus. According to Stranges (1984), J.J. Thomson - without bothering to justify his thesis - proposed the idea that electrons could easily migrate from one atom to another, thus generating positive or negative ions capable of mutual electric attraction. Thus, ideas behind Berzelius's theories were retrieved to some extent, with the main difference that the new theory referred to the sub-atomic level instead of the macroscopic level (Stranges 1984). Gravitational force between atoms, originally proposed by Frankland and quickly abandoned, is here replaced by Coulomb forces between oppositely charged particles, i.e. subatomic components.

The electrical or electrostatic theory of chemical bonding had many supporters: O. Lodge (1851-1940), J. Stark (1874-1957), W. Ramsey (1852-1916), R. Abegg (1869-1910) e W. Kossel (1888-1956). In his 1903 monograph entitled *Modern views on Matter*, Lodge wrote:

“It becomes a reasonable hypothesis to surmise that *the whole of the atom may be built up of positive and negative electrons interleaved together*, and of nothing else; an active or charged ion having one negative electron in excess or defect, but the neutral atom having an exact number of pairs. The oppositely charged electrons are to be thought of on this hypothesis as flying about inside the atom, as a few thousand specks” (Lodge 1903 cited by Stranges 1984, italics added).

Johannes Stark in a 1903 publication entitled *Die Dissoziierung und Umwandlung chemischer Atome* stated that chemical union was the sharing of one electron between two atoms, in a molecule. He represented sharing with electric lines of force going from the electron towards each bound atoms, as shown in Figure 3.7. If atoms have different electronegativity, the interaction of the electron with the atomic pair is asymmetrical (Stranges 1984).

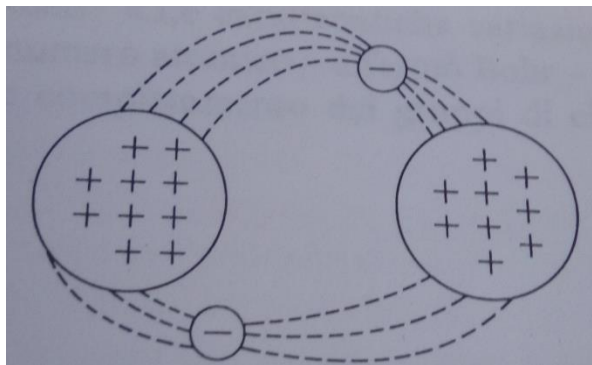


Figure 3.7 Diagram of the representation of the chemical bond according to Stark: the lines of force of the valence electron deviate in part from their positive sphere to that of the atom to which it binds (Solov'ev 1976).

In 1908, W. Ramsay tried interpreting the structure of some compounds, either simple or complex, through the electronic theory. Ramsey proposed to describe atoms as spheres: within them, electrons moved around a positively charged central nucleus. He also proposed to distinguish two sets of electrons: constitutive electrons (i.e. those held more tightly) and valence electrons (i.e. those held less tightly). In fact, he introduced the notion of atomic core, which later would be crucial in Lewis' model. Ramsay was also recognized by Lewis as the first to suggest electron sharing between atoms (Solov'ev 1976 p. 392). In the frame of his electrical theory of chemical bonding similar to Thomson's, the German chemist Richard Abegg proposed the *theory of eight*: he postulated that each element exhibits highest positive and negative charges, whose sum is 8 (Abegg 1904). The highest positive charge for a given element equals the group number of the element. Furthermore, according to Abegg, atoms had 1 to 8 electrons available for bonding: positive charge was due to electron loss and equals the number of bond electrons that would bring atoms back to neutrality. Abegg's publications are the first reporting the number of electrons available for bonding (Jensen 1984; Stranges 1984). In all these writings, there is a constant reference to periodicity of 8, which had been highlighted by D.I. Mendeleev (1834-1907) in his periodic table, and by Newlands in his *octave law*. In 1871, while he was investigating periodicity, Mendeleev proposed two rules related to atomic valence, where the number 8 had a key role. He stated that the highest possible valence of any element of the Periodic Table was 8 (first rule) and that the sum of positive and negative¹⁰ valence of an element was 8 (second rule, Figure 3.8) as is the case of chlorine in compounds HCl and Cl₂O₇ (Jensen 1984).

Hydride RH _n	Oxide R ₂ O _{8-n}
CH ₄	C ₂ O ₄ ≅ CO ₂
NH ₃	N ₂ O ₅
SH ₂	S ₂ O ₆ ≅ SO ₃
ClH	Cl ₂ O ₇
none	OsO ₄

Figure 3.8: Mendeleev's Second Rule (Jensen 1984)

In 1916, Kossel - a German physicist - attempted to extend Abegg's theories. His studies confirmed both Abegg's and Thomson's theories; they supported the idea that electron transfer between atoms was related to the achievement of complete electronic shells similar to noble gases' configuration (Jensen 1984). In fact, Kossel formulated the octet rule for ionic compounds; he recognized that atoms of various elements tend to gain or lose electrons so to get the same number of electrons as inert gases (Gillespie 2006). The first two decades of the twentieth century were therefore dominated by theories that postulated the existence of charged

¹⁰ Positive valence refers to bound oxygen atoms; negative valence refers to bound hydrogen atoms

- 2) every atom contained one or more nearly weightless, negatively charged particles called electrons;
- 3) every atom contained a second kind of particle, considerably heavier than the electron, that accounted for most of the atom's mass and had sufficient positive charge to balance the electron's negative charge;
- 4) the transfer of electrons produced the attractive force holding atoms together.

3.1.7 Lewis-Langmuir theory of bonding

The connection between electrons and chemical bonding stated in point 4 paved the way to a new and alternative theory. A crucial step in the evolution of bonding ideas occurred in 1916, when Gilbert N. Lewis (1875-1946) developed a model based on a completely new concept: shared electron pairs (Lewis 1916; Hendry 2008; Ducamp 2014). We already mentioned that the idea of electron sharing between atoms circulated in the chemical community and preceded Lewis's theory: Lewis himself attributed this idea to Ramsay. According to Solov'ev (1976 p. 393), the first to launch this hypothesis was N.A. Morozov, in the Russian text entitled *Periodic systems of the structure of substances. Theory of the formation of chemical elements*, published in 1907 in Moscow. Morozov proposed the existence of two distinct types of bonds, which actually anticipated the covalent and ionic bonding models (Solov'ev 1976 p. 394).

Back to Lewis, in his renowned article published in 1916 in the *Journal of the American Chemical society*, he reminds the different properties of 'polar' and non-polar compounds and provides the following explanation:

“the essential difference between the polar and the non polar molecule is that, in the former, one or more electrons are *held by sufficiently weak constraints so that they may become separated from their former positions in the atom, and in the extreme case pass altogether to another atom*, thus producing in the molecule a bipole or multipole of high electrical moment. Thus in an extremely polar molecule, such as that of sodium chloride, it is probable that at least in the great majority of molecules the chlorine atom has acquired a unit negative charge and therefore the sodium atom a unit positive charge, and that the process of ionization consists only in a further separation of these charged parts” (Lewis 1916, italics added).

This excerpt describes what we now call ionic bond, found in “extremely polar molecules” such as that of sodium chloride. Interestingly, sodium chloride is not yet designed as ‘ionic substance’ and the notion of molecule prevails. Lewis then describes ‘non polar’ molecules:

“If then we consider the nonpolar molecule as one in which *the electrons belonging to the individual atom are held by such constraints that they do not move far from their normal positions*, while in the polar molecule the electrons, being more mobile, so move as to separate the molecule into positive and negative parts, then all the distinguishing properties of the two types of compounds become necessary consequences of this assumption, as we may readily show. Thus polar compounds with their mobile parts fall readily into those combinations which represent the very few stable states, while the nonpolar molecules, in which the parts are held by firmer constraints, *are inert and unreactive*, and can therefore be built up into the numerous complicated structures of organic chemistry” (Lewis 1916, italics added).

Lewis's idea that electron sharing, instead of electron transfer, could take place between atoms, depending on how tightly electrons were held overcome the need for oppositely charged entities hold together by Coulombic forces. Interestingly, in Lewis's own words, electron sharing reflects on chemical reactivity. This hypothesis was able to explain the experimental evidence that ions are not found in organic substances: it allowed

overcoming the limitations of the positive-negative theory when applied to non-polar compounds. Lewis thought that non-polar and ionic compounds were extremes outcomes of the same bonding mechanism: electron pair distribution could be completely symmetric (in non-polar compounds) or completely asymmetric (in ‘polar’ compounds, where the electron pair is localized on one of the two bound atoms which becomes negatively charged, whereas its counterpart was positively charged). So, the positive-negative theory (which implies ion formation) became a special case of the more general Lewis theory. Lewis refused a dualistic view of bonding (polar vs. non polar as two radically distinct categories). In his view, chemical bonding was characterized by distinct degrees of polarization:

“However, according to the theory which I am now presenting, it is not necessary to consider the two extreme types of chemical combination, corresponding to the very polar and the very non polar compounds *as different in kind, but only as different in degree*” Lewis 1916, italics added).

In the same article, Lewis states the 6 postulates of the theory of cubical atom, which include the famous *rule of eight* (3rd postulate):

“1. In every atom is an essential kernel which remains unaltered in all ordinary chemical changes and which possesses an excess of positive charges corresponding in number to the ordinal number of the group in the periodic table to which the element belongs.

2. The atom is composed of the kernel and an outer atom or shell, which, in the case of the neutral atom, contains negative electrons equal in number to the excess of positive charges of the kernel, but the number of electrons in the shell may vary during chemical change between 0 and 8.

3. The atom tends to hold an even number of electrons in the shell, and especially to hold eight electrons which are normally arranged symmetrically at the eight comers of a cube.

4. Two atomic shells are mutually interpenetrable.

5. Electrons may ordinarily pass with readiness from one position in the outer shell to another. Nevertheless, they are held in position by more or less rigid constraints, and these positions and the magnitude of the constraints are determined by the nature of the atom and of such other atoms as are combined with it.

6. Electric forces between particles which are very close together do not obey the simple law of inverse squares which holds at greater distances” (Lewis 1916).

The first two postulates establish the distinction between electrons of inner shells, i.e. *core* electrons, and electrons of the outer shell of atoms. This distinction has little relevance from the physical viewpoint, but it is crucial from the chemical point of view. In fact, *core* electrons belong to the atomic *kernel*, which keeps unperturbed during chemical transformation: chemical bonding involves only outer shell electrons. The idea that chemical bonding and bonding modes are determined by the properties of these outer shell electrons proved valid for the development of the bonding models still used today.

In those same years, W. Kossel found that valences of lighter elements were intimately connected with the formation of electron octets (third postulate). The Lewis-Kossel description of ionic bonding encompassed two central chemical concepts. First, formation of ions with electronic configurations equal to those of noble gases results in isoelectronic series. For example, ions Al^{3+} , Mg^{2+} , Na^+ , F^- , O^{2-} and N^{3-} are all isoelectronic with the atom of Ne. Furthermore, compounds formed by isoelectronic ions are almost always isostructural. In fact, crystals of two isosteric compounds such as NaF and MgO have both a face-centered cubic structure. Second, Lewis and Kossel recognized that the similar chemical properties manifested by elements belonging to the same group depended on the number of valence electrons, as inner electrons do not concur in

determining the reactivity of chemical elements. For example, the two series of compounds LiF, NaF, KF, CsF, RbF and KF, KCl, KBr, KI have the same minimum formula and the same structural features because they share the same number of valence electrons (1 in metals, 7 in halogens). The description of the ionic and covalent bonding models made by Kossel and Lewis strengthened the structure of the periodic table proposed by Mendeleev and provided a causal explanation rooted in valence electrons (Mingos 2019).

Lewis's theory required exactly two electrons to form a chemical bond as a direct consequence of Lewis' static atomic model. Lewis hypothesized that electron pairs sharing allowed justifying structural formulas of compounds. Representations of atoms according to the cubical atomic model are shown in the figure below:

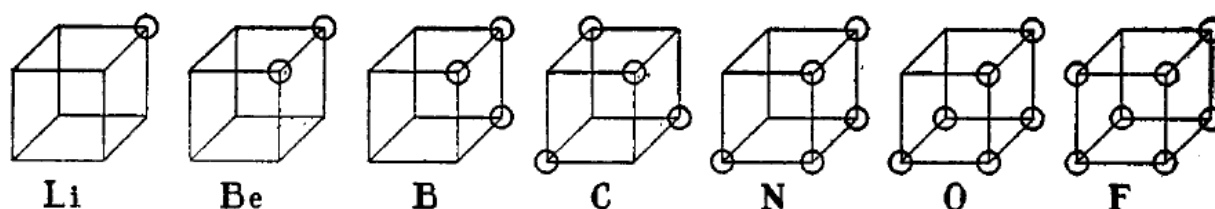


Figure 3.10: atoms of first period elements of the periodic table according to the Lewis model (Lewis 1916)

The circles represent the electrons of the outer shell of neutral atoms. Based on these representations and the six above-mentioned postulates, Lewis was able to justify many aspects of chemical bonding. He found that the number of outer shell electrons in very many molecules was always an even number and often a multiple of 8 (Figure 3.11):

Number of Valence Electrons in Atom	Total Number of Valence Electrons in Molecule
N = 5	
H = 1	NH ₃ = 8
C = 4	
H = 1	CH ₄ = 8
C = 4	
O = 6	CO ₂ = 16
S = 6	
O = 6	SO ₃ = 24
C = 4	
Cl = 7	CCl ₄ = 32

Figure 3.11: number of valence electrons in individual atoms and total number of valence electrons in molecules (Stranges 1984)

Lewis argued that this was because each atom in the molecule shared a pair of electrons with another atom to which it was bound:

“the simplest explanation of the predominant occurrence of an even number of electrons in the valence shells of molecules is that *the electrons are definitely paired with each other*” (Lewis 1923, cited by Gillespie 2006, italics added)

In this description Lewis includes non-bonding electrons and states that this corresponds to the situation where 8 outer shell electrons occupy the 8 vertices of a cube:

“the most stable condition for the atomic shell is the one in which eight electrons are held at the corners of a cube” (Lewis 1916).

Let's consider the formation of chemical bonds in the diiodine molecule (Figure 3.12), as described by Lewis:

“But at the same time *an electron of the second atom may fit into the shell of the first, thus satisfying both groups of eight* and giving the form C which is the predominant and characteristic structure of the halogens” (Lewis 1916).

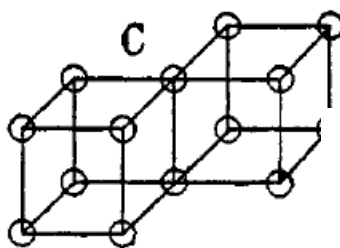
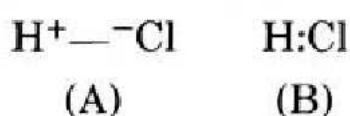


Figure 3.12: Representation of the molecule of a halogen according to the Lewis cubic atom model (Lewis 1916, italics added)

To expose his theory, Lewis adopted a new symbolism, the so-called Lewis structural formulas (Figure 3.13). In these formulas, electrons (represented by dots) were distributed around the symbol of the element. Two points laying between two adjacent atoms represented a shared pair of electrons, i.e. a chemical bond:



(A): in accordance with the positive-negative theory

(B): in accordance to Lewis' shared electron pair theory

Figure 3.13: Lewis structure of hydrochloric acid (Stranges 1984)

The theory was successful among chemists: this is proved by the fact that 10 years after the publication of Lewis' article, his theory was already widely accepted and applied by the chemical community (outstanding chemists such as F. Russell von Bichowsky, Joel Hildebrand, Wendell Latimer, Worth Rodebush, and Robert N. Pease applied Lewis theory in their research) (Stranges 1984). The greatest supporter of the Lewis theory was Irving Langmuir (1881-1967), who contributed spreading it in the United States and abroad, to the point that the theory was renamed after him (Langmuir or Lewis-Langmuir theory): this generated a controversy between the two scientists as regards to the authorship of the theory itself. The 1921 article entitled "Types of Valence" was the last relevant work that Langmuir devoted to the octet theory (Jensen 1984). Langmuir first distinguished valence into three different types:

“From the theory proposed by G.N. Lewis in 1916 and subsequently extended by the writer, it is clear that the term *valence* has been used in the past to cover what we may now recognize as three distinct types of valence, viz.:

1. Positive valence: the number of electrons an atom can give up.
2. Negative valence: the number of electrons an atom can take up.
3. Covalence: the number of pairs of electrons an atom can share with its neighbors.”

(Langmuir 1921)

The author remarks that his reference points are:

- the Rutherford model of the atom;
- Coulomb forces acting between the charged particles inside atoms;
- The fact that electrons do not collapse on the atomic nucleus of the atom due to repulsive forces.

In his 1921 work, Langmuir postulates that:

- 1) electrons in atoms are distributed around the nucleus in successive layers containing 2, 8, 8, 18, 18 and 32 electrons, respectively;

- 2) two atoms may be coupled together by one or more doublets held in common by the completed sheaths of the atoms;
- 3) the residual charge on each atom or group of atoms tends to a minimum.

The term *residual charge* means the total charge of an atom or group of atoms regardless of its sign. It often happens that the tendency expressed by postulate 1 prevails against that expressed by postulate 3. This occurs in salts: in fact, postulate 3 predicts that neutrality would be the most stable condition. On the other hand, postulate 1 predicts the stability of full electrons layers. Hence, in sodium chloride both postulates are satisfied by the formation of single charged ions (Na^+ and Cl^- ions exhibit full outer shells and the lowest possible electric charge). In some cases, such as for example in the SF_6 compound, the high charge of sulfur (+6) contradicts postulate 3, but is admissible thanks to the high electronic affinity of fluorine. Conversely, in molecular compounds such as CH_4 , NH_3 , H_2O and HF the tendency of the first postulate and that of the third coincide. Langmuir remarks:

“Thus in any group of atoms Postulates 1 and 3 are both completely satisfied if the covalence of each atom is equal to the negative valence of that atom” (Langmuir 1921).

Thus in each atom of the aforementioned compounds the covalence is equal to the negative valence (whose values are 4, 3 and 2 for carbon, nitrogen and oxygen respectively, while it assumes the value 1 for both hydrogen and halogen) so that the residual charge on each atom is zero. In this seminal work, Langmuir proposes a classification of compounds based on the first postulate: compounds which comply with the first postulate, compounds which don't, and exceptions. Compounds that comply with the first postulate (i.e. what we now call the octet rule) contain atoms that fill their outer shells in two alternative ways:

“A given group of neutral atoms can interact to complete their sheaths in two ways:

1) By transfer of electrons.

- a. atoms having sheaths containing only a few electrons may give up these extra electrons to other atoms.
- b. atoms having nearly complete sheaths may take up electrons from other atoms.

2) By sharing doublets.

Atoms can share doublets with other atoms and thus complete their sheaths with fewer electrons than would otherwise be necessary” (Langmuir 1921).

Compounds which do not comply with postulate 1 “are compounds in which some of the electrons are not arranged in complete layers or sheaths, so that the tendency of Postulate 1 is not completely satisfied” (Langmuir 1921). This type of compounds includes metallic substances, characterised by ‘free’ electrons:

“The “free” electrons which are thus compelled to remain in incomplete sheaths are responsible for the metallic properties shown by all electropositive elements in the solid or liquid state” (Langmuir 1921).

Furthermore, Langmuir identifies a category of compounds that, basically, include what we now classify as ‘exception to the octet rule’.

Langmuir puts the same emphasis as Lewis on the role of outer electron shells:

“The sheath of any atom (or atomic ion) consists of all the electrons in the outside layer provided that this layer is incomplete when the atom is electrically neutral. Thus atoms of the inert gases (neon,

argon, etc.) and ions such as Na^+ , Ca^{++} , etc., have no sheaths for the outside layers of these atoms consist of electrons which already form a complete layer in the neutral atom” (Langmuir 1921).

Noble gases are the only elements whose uncombined atoms exhibit full shells: therefore, they do not possess a valence shell. Only atoms whose outer shells are incomplete tend to satisfy the first postulate, by rearranging their electrons:

“When as the result of such rearrangement of electrons, the sheath of an atom has become complete, we may speak of the atom like *a complete atom*. Similarly, in the interaction between atoms leads to complete satisfaction of the tendency of Postulate 1, so that all the atoms become complete, we may say that a complete compound is formed” (Langmuir 1921).

This is the main cause for chemical reactivity that results in the formation of new compounds. Whenever the rearrangement of electrons results in the formation of *incomplete atoms*, we are faced to what we would now define as *exceptions to the octet rule*.

In 1923, the controversy between Lewis and Langmuir prompted Lewis to publish a monograph entitled *Valence and the Structure of Atoms and Molecules* which tackles the problem of double and triple bonds in molecules. This is a foundational chemistry text, where Lewis’ theory of acids and bases is also reported.

Despite its explanatory power, Lewis’s theory also had some theoretical weaknesses. The main problem raised by the concept of electronic doublet, proposed by Lewis, arose from its disagreement with the laws of electrostatics. How to explain the fact that two negative charges did not repel each other, but rather turned out to be coupled? Lewis was aware of this limitation and mentions it in the 1916 article, where he states that electrons could pair up “perhaps by magnetic force, if the magneton theory is correct, or perhaps by other forces which become appreciable at small distances”. The final answer to the problem came in subsequent years, with the birth of quantum mechanics and, in particular, with the concept of electron spin. Quantum mechanics provides a complex interpretation of chemical bonding starting based on the idea of the double wave-corpuscular nature of matter. According to this type of mechanics, the microscopic and sub-microscopic components of matter are described as wave phenomena. The electron, described as a wave, is represented by the differential equation of Erwin Schrödinger (1887-1961), whose solutions are mathematical functions, called orbitals, describing the possible energy states of electrons in the atom. The notion of orbital thus replaced the concept of orbit, still found in Bohr’s atomic model. Orbitals are associated with 4 quantum numbers designated with symbols n , l , m_l and m_s . The last quantum number, the spin number, solved the question of electron coupling, because it allows justifying the fact that two mobile entities, bearing the same charge, can give rise to energetically favorable interaction. In fact, two electrons of opposite spin may couple, as predicted by Pauli exclusion principle (1925): distinct electrons cannot share the same set of 4 quantum numbers; therefore, the spin number of two paired electrons has to be different. According to this principle, the shared electron pair in Lewis’ model of chemical bonding find its justification (*a posteriori*) in quantum theory: Lewis’ electron pair is described by two electrons, sharing 3 quantum numbers and differing only on the 4th, i.e. spin number. With the birth of quantum chemistry, the description of chemical bonding changes radically, as bonding is conceived as a quantum-mechanical phenomenon. This implies shifting from a deterministic description (based on the possibility of localizing a particle in the three-dimensional space and time) to a probabilistic description, deriving from Heisenberg’s uncertainty principle (1901-1976), which led to the definition of the concept of probability density. The electron must therefore be imagined as a wave propagating in space and no longer as a particle placed at a given point along an orbit. Consequently, bonding becomes a wave interference figure. Quantum mechanics was a fundamental step forward in the treatment of the bonding problem: this approach prevailed very quickly on previous theories within the chemical community. However, it is worth remarking that chemists still use those aspects of previous theories still

endowed with heuristic, operational and representative value. For example, Lewis structures and symbols are still found in the representation of synthesis and reaction schemes in organic chemistry. In fact, quantum mechanics uses a cryptic language, a rather complex mathematical apparatus and provides a description of the atomic and subatomic world that is virtually not representable. Conversely, the deterministic and corpuscular view of the atomic and subatomic world is still useful to chemists as it helps assigning meanings to the highly abstract conceptual apparatus of quantum chemistry. Linus Pauling (1901-1994) from the 1930s onwards applied quantum mechanics to address the problems related to chemical bonding (Hendry 2008) and in 1928 he proposed the new concept of hybrid orbital which became part of the theory of valence bond (VB). This theory is, *de facto*, a translation of Lewis theory in quantum terms: in fact, chemical bonding according to the VB theory is the linear combination of atomic orbitals that results in a wave function that describes electron sharing by taking into account the possibility of exchange between two paired electrons). Thus, the VB theory is based on monocentric orbitals, i.e. orbitals centered on single atoms, deriving from linear combinations of the orbitals of isolated atoms; it is able to account for the directionality typical of covalent bonds. This theory was then almost replaced by molecular orbitals theory (MO), introduced by F. Hund (1896-1988) and R. Mulliken (1896-1986) in the 1950s. The MO theory adopts a radically distinct perspective on molecules: these become integrated systems, wherein the original atoms do not actually survive (the system of orbitals of isolated atoms undergoes a radical transformation once bonding occurs). Furthermore, the MO theory implies the construction of multicentric molecular orbitals, i.e. centered on all the nuclei in the molecule, resulting from linear combination of atomic orbitals (Villani, 2001 p. 109). This implies conceiving molecule as systems wherein all atoms interact with each other, albeit to different extent: bonding is spread over the entire molecule.

Paulings' VB theory provides a theoretical foundation for the *rule of eight* enunciated by Lewis (valid at least for the lighter elements of the Periodic Table):

“The shared electron structures assigned by Lewis to molecules such as H₂, F₂, Cl₂, CH₄, etc., are also found for them by London. The quantum mechanics explanation of valence is, moreover, more detailed and correspondingly more powerful than the old picture. For example, *it leads to the result that the number of shared bonds possible for an atom of the first row is not greater than four*, and for hydrogen not greater than one, for, neglecting spin, there are only four quantum states in the L-shell and one in the K-shell” (Pauling, 1928 cited by Stranges 1984, italics added).

Hendry remarks that Pauling linked the principles of quantum mechanics to Lewis' static electronic structures: he reinterpreted the notions of bond directionality and resonance typical of organic compounds structures, in a quantum-mechanical perspective (Hendry 2008). It is worth underlining that the quantum-mechanical description of bonding made by Pauling's VB theory does not reflect a purely physical thought: it is justified by chemical evidence, as is Lewis' model to which VB theory refers continuously. In the 1960 edition of "The Nature of the Chemical Bond", before going into the quantum-mechanical description of chemical bonding, Pauling provides a very clear and effective definition:

“We shall say that there is a chemical bond between two atoms or groups of atoms in case that the forces acting between them are such as to lead to the formation of an aggregate with sufficient stability to make it convenient for the chemist to consider it as an independent molecular species” (Pauling 1960 p. 6).

This definition reminds us that the treatment of the chemical bond cannot neglect energetic aspects. In fact, the condition for chemical bonding is the achievement of a balance between attractive and repulsive interactions acting in the system, which coincides with the formation of an energetically stable aggregate (an independent molecular species). Pauling points out that this definition does not refer exclusively to covalent

bonding in organic molecules, but also ionic bonds in salts and even weak intermolecular forces, whose energetic content is sometimes comparable to chemical bonds (Pauling 1960 p. 6). This statement is relevant because it is common to treat intramolecular and intermolecular bonds dichotomically, as if these phenomena had radically distinct physical basis. On the other hand, Pauling's excerpt strengthens the idea that the notion of bond has distinct disciplinary meanings: a *chemical meaning*, which justifies the need for various models in relation to the experimental behaviors that need to be explained (reactivity, chemical-physical properties of the substances); a *physical meaning*, which considers bonds as physical interactions between atoms, distinguished by the *amount of bonding energy* involved. The stability of the resulting aggregates depends on the energy involved, no matter if these aggregates are molecules or physical states. Despite their difference, both aspects must be reconciled and coexist in the didactic treatment of the concept of bond. Finally, Pauling clarifies the nature of the concept of bond, through a definition that demonstrates his strong epistemological awareness:

“*Bonds are theoretical constructs*, idealizations, which have aided chemists during the past one hundred years in developing the convenient and extremely valuable classical structure theory of organic chemistry” (Pauling 1970 p. 999)

Pauling reminds that bonds are not entities, but theoretical constructs aimed at designing relationships between atoms. These relationships have a deep chemical meaning, as they allow articulating the central problem of chemistry, that is, to clarify the relationship between structure and reactivity of substances.

3.2 Conclusions

This survey of the history of the notion of chemical bond and its related concepts brings to light various aspects that are relevant to chemical education. First of all, the knowledge - even a superficial knowledge - of the history of the foundational ideas of a discipline allows identifying:

- i) the reasons behind the birth of new concepts.
- ii) the evolution of these concepts.
- iii) the inter-relations between different concepts.

This knowledge informs didactic transposition, in that it highlights the conceptual prerequisites necessary for achieving full comprehension of chemical bonding (e.g., what comes first, the notion of bonding or the notion of molecule? what is the connection between bonding and molecular structure?).

The historical excursus outlined in the previous pages reveals the difficulties inherent in the formalization of a concept – the bonding concept – that expresses a relationship, and more precisely a *privileged relationship between atoms*. This relationship has a deep chemical meaning, as chemists use it to provide interpretations (at the microscopic level) of macroscopic properties of substances, ranging from physical properties (melting and boiling points, solubility, etc.) to reactivity (i.e. possibility of transforming one substance into another).

The history of scientific ideas shows that the modern notion of chemical bonding arises from the much more nuanced concept of affinity. Chemical affinity, a concept borrowed from the philosophical and alchemical domain, was an attempt to rationalize macroscopic evidence: substances do not combine or react randomly, not everything combines with everything, but there are preferential combinations and constraints. The concepts of valence and structure arose to rationalize the nature and origin of these constraints. The notion of chemical bonding informs the notion of molecule (intended as a stable aggregate of atoms, expressed by a brute formula): a molecule is an ordered aggregate, in which atoms interact in a specific, directional way. A molecule is therefore an entity with a structure. The constraints that determine the molecular structure derive

from the elements found in molecules, that are characterized by a precise combinatorial capacity (*valence*) and by different properties (e.g. acidity or basicity, metallic or non-metallic character, electronegativity, etc.). This set of concepts allows accounting for the different properties exhibited by substances at the macroscopic level; it also correlate these properties with those of the elements that constitute them (electronegativity, electronic affinity, etc.). The various bonding models and atomic models are an attempt to rationalize the origin of the electrical properties of matter.

The history of chemical bonding clarifies what is rarely highlighted in chemistry courses, despite its didactic relevance: the distinction between concept and model. The notion of chemical bond lies upstream from descriptive models: they do not coincide with each other. We may say that the concept expresses a '*philosophical*' need (the need to give a face to a privileged relationship between atoms); conversely, models express a '*practical*' '*scientific*' need (that of characterizing the concept and making it operational, i.e. by constructing explanatory schemes and making predictions on the experimental behavior of substances).

Another aspect of great educational importance highlighted by the historical survey is the disciplinary interweaving between chemistry and physics that allowed developing valid bond models. Such intertwining highlights some aspects that should be borne in mind by teachers:

- The descriptive basis of chemical bonding is physical, as it hinges on electromagnetism. An integrated treatment of this topic in the chemistry and physics teachings is then desirable. In fact, in the usual teaching practice, chemical bonding is addressed by the chemistry teacher without contributions by the physics teacher. A true interdisciplinary approach between these two disciplines, formalized in schools' teaching plans, would allow the proper construction of bonding models through the application of physical laws and notions such as electric charge, electric field and Coulomb's law. Furthermore, such a practice would comply with conceptual pre-requisites; it would also allow rationalizing teaching time schedules and increase the effectiveness of the teaching action. The so-called 'integrated sciences' in the first biennium of Italian high schools (which include chemistry, physics and biology) would allow, if properly designed, a synergistic action capable to avoid an excess of fragmentation in the teaching/learning of scientific disciplines, showing their interdependence. The didactic transposition of the concept of chemical bonding provides the opportunity of realizing this purpose.
- The traditional distinction between intra- and inter-molecular bonds is justified exclusively at the chemical level. It is chemistry that needs to differentiate between *internal* relationships to molecular entities and relationships *between* molecular entities. This happens because the notion of substance is a foundational chemical notion, as chemistry qualifies as a discipline that investigates the transformation of substances. Conversely, at the physical level, intra- and inter-molecular interactions differs only as regards to their energy scales. In fact, physics relies on the notion of matter: the differentiation of matter into substances is secondary, in physics. An integrated (chemical and physical) approach to the concept of bonding would, on one hand, allow highlighting the continuum of interatomic bonding forces, on the other hand, make students understand the meaning of distinct types of interatomic bonding models.

This survey of the historical-epistemological evolution of the concept of chemical bonding and its related notions (valence, electronegativity and structure) allowed discussing the origin of a few key-concepts (Figure 3.14) and of the explanatory models of bonding. The identification of the historical paths that led to the elaboration and evolution of the concepts of chemical bond and its correlates is fundamental to make informed didactic choices (Figure 3.14) and to identify the learning objectives that it is realistic to pursue at any school

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Chapter 4

A teaching sequence on the concept of interatomic bonding

Introduction

The teaching-learning sequence on the concept of interatomic bonding presented in this chapter is based on the results of a literature survey that brought into light various critical issues of at the epistemological, didactic, cognitive levels.

Some of the main critical issues that we identified and we took into account in designing our teaching sequence are summarized below:

- ✓ **The multiplicity of models used for describing the bonding phenomenon:** the concept of interatomic bond is an abstraction, that faces a cognitive and descriptive need raised by the wide range of chemical-physical properties of substances. It is subject to various types of description, that is, to a very articulated modelling description. The bonding notion can be approached through different theoretical frameworks (e.g. quantum approach, DFT density functional theory, electrostatic approach, etc.), within which various types of models are developed. The covalent, ionic, hydrogen bridge, etc. bonding models are theoretical tools able to interpret the variety of macroscopic properties and reactivity of chemical substances: hence they are called upon to satisfy the need of interpreting the behaviour of the physical realm. However, in the teaching practice, they are usually introduced without clarifying their character of theoretical and interpretive tools, justified by a theory and rooted into the material reality. Furthermore, their treatment lacks of unity: the (general) concept of bond is overshadowed by the variety of descriptive models, conveying the idea of a fragmented and incoherent explanatory framework, that makes it impossible to grasp the relationships of continuity existing between different bonding models. In other words, the didactic transposition of interatomic bonding does not usually make reference to unifying principles, i.e. a coherent conceptual framework (Nahum et al. 2010, Joki e Aksela 2015 e 2018). Various problems arise from this: i) the meaning of the bonding phenomenon is not grasped by students; ii) students tend to overlap the physical realm and its descriptive models; iii) the reasons why one single bonding model is insufficient are not understood, and the common features to the various models are not understood. Hence, misconceptions are developed, such as the transfer of macroscopic properties to microscopic particles or the application of the notion of molecule to any substance. Didactic research on the concept of chemical bond highlights some basic needs: i) to clarify the nature and function of scientific models and the relationship they have with reality; ii) to educate students to distinguish between perceptual facts and explanatory models (an essential aspect of science teaching and learning); iii) to understand the meaning of the bonding notion, with all its implications.
- ✓ **The relationship between macroscopic and microscopic levels:** the concept of interatomic bonding pertains to a level of reality (atomic-molecular and nuclear-electronic) inaccessible to perception, but it justifies the onset of observable properties in substances (macroscopic level). These chemical-physical properties are interpreted in terms of interaction between microscopic entities. Following Johnstone's lesson (2010), we found appropriate (at both the epistemological and didactic level) to let the sequence start from the analysis of a range of chemical-physical properties of substances (macroscopic level). The questions raised by this variety of phenomena call for the development of a theoretical framework that allows justifying facts such as: the physical states of substances at a given temperature and pressure; the water solubility/insolubility of substances; their electrical or thermal

conductivity, etc. The symbolic aspects are also fundamental and find space in the vast iconographic apparatus used to represent interatomic bonds. The symbolic language can feed various misconceptions, such as the materialization of bonds.

- ✓ **Models that rely on very advanced formalisms are scarcely understood by secondary school students:** some scholars (Joki et al. 2015; Nahum et al. 2008 and 2010; Dhindsa and Treagust 2014), remark that the use of quantum models is inappropriate at school, because students do not possess the mathematical and cognitive tools necessary for understanding these models and their related formalisms. Besides, quantum concepts are often misunderstood even by teachers (Bergqvist et al. 2017). The result is a simplistic didactic transposition, which becomes a vehicle for misconceptions (e.g. the identification of the orbital with a region of space) that are difficult to eradicate in subsequent school contexts.
- ✓ **A generalized lack of awareness of the historical evolution of concepts and models by teachers:** several scholars (Joki and Aksela, 2018; Ünal et al. 2006) remark the insufficient knowledge of the history and evolution of scientific concepts by teachers of scientific subjects; they also complain about the absence of historical-philosophical paths in chemistry texts. To know the historical paths that led to the elaboration and evolution of concepts opens to its didactic exploitation, not in a purely narrative fashion, but in the epistemological perspective. The historical-epistemological approach applied to the notion of interatomic bonding allows highlighting the conceptual knots that students will have to face during the learning process and to design ad hoc problem-situations
- ✓ **The most common alternative conceptions:** when the didactic transposition of the concept interatomic bonding does not pay attention to the various aspects highlighted above, students inevitably develop alternative conceptions (Tsaparlis et al. 2018; Erman Erman, 2016; Othman et al. 2008; Ünal et al. 2006; Coll et al. 2001).

Here are some common alternative conceptions related to the concept of interatomic bonding:

- Interaction phenomena between charges are considered relevant only for ionic bonding
 - The physical nature of intra- and inter-molecular bonds is perceived as radically distinct: the role played by electrons in both cases is not understood
 - The meaning of inter- and intra-molecular bonds is not caught, their models and role are mixed up
 - Physical phenomena (e.g. change of physical states) are associated with the breaking of covalent bonds
 - Ionic and metallic compounds are thought as molecular substances
 - The role of molecular geometry in determining the polarity of a molecule is not understood (e.g. students claim that a molecule containing polar bonds is always polar, regardless of its geometry).
- ✓ **The conscious use of digital tools for representing matter at the microscopic level:** the high degree of abstractness of the interatomic bonding notion makes its mental representation difficult, mainly because the atomic-molecular and nuclear-electronic world belongs to a virtually unrepresentable level of reality (the quantum level).

On the other hand, the use of iconographic and/or verbal representations based on analogies or metaphors is essential to develop reasoning at the atomic and subatomic levels, and to assign meanings. The use of digital tools and dynamic iconographic representations (animations, simulations, model representations) made possible by information technology can support the teaching of interatomic bonding (Patron et al. 2017; Frailich et al. 2009).

These representations allow highlighting dynamic aspects that a static 2D image cannot render; in this way, they concur in building up links between the macroscopic and microscopic levels. According to

Frailich et al. (2009), the use of ICTs may even support the social dimension of learning, which can be enhanced by a guided and conscious use of ICTs whenever online activities are carried out in small groups.

Finally, the use of digital tools has a motivational value, given the role played by technology in the daily life of students. Obviously, great caution is needed: the teacher must make critical choices consistent with the didactic objectives to be pursued. In fact, the extreme confidence of students in the computer world can amplify the evocative power of incorrect images and metaphors and foster further misconceptions.

In addition to the above-mentioned points, our teaching sequence was designed according to the following criteria:

- ✓ **Socio-constructivist approach to learning:** the two basic assumptions of this approach are: i) a non-transmissive conception of learning: knowledge is the product of the learner's activity, students play an active role in learning; ii) the construction of knowledge is a social process: discussion among students and sharing of ideas are essential parts of the learning process.
- ✓ **Attention paid to conceptual prerequisites and recursive use of concepts:** experts in science education recommend that the introduction of new concepts always respond to the emergence of new explanatory and interpretative needs. New notions must not be introduced apodictically. In addition, the construction of new concepts necessarily rests on the knowledge already possessed by students: “Scientific concepts cannot be assimilated once and for all and in a final form; the construction of concepts takes place progressively, in the course of a development that passes through different registers or levels of conceptualization, gradually more formal and more general” (Roletto, 2005). The sequence proposed here is therefore configured as a logical chain, built according to precise conceptual prerequisites, and based on some unifying concepts. In the sequence, new concepts and models are constructed or recalled (and made evolve) whenever the previous knowledge does not satisfy the explanatory needs raised by new phenomenon: different bonding models are then gradually introduced or modified.
- ✓ **Circular approach (from the macroscopic level to the microscopic and back):** it is the world of phenomena (macroscopic level) that raises questions that call for new interpretive models. In chemistry, models lie at the microscopic level. In turn, models allow making predictions that must be verified at the macroscopic level. Hence the endless coming and going between these two levels of reality, mediated by the symbolic language.
- ✓ **Use of a conceptual approach based on electrostatic interactions:** the whole sequence is built on the physical concept of interaction between charges, which represent the element of continuity between bonding models and the conceptual backbone of the sequence itself. We have therefore deliberately chosen to limit the use of concepts belonging to the quantum world to a minimum. This choice is suggested by the outcome of didactic research (Joki e Aksela 2015, 2018; Bergqvist et al. 2016): i) the non-coincidence of the learning needs of secondary school students and the explanatory needs of scholars belonging to the chemical community; ii) the need to rely on models that are intelligible to students (i.e. models based on phenomena and concepts that are part of students' knowledge) and to focus on the construction of meanings; iii) the consideration that models that disciplinary research considers outdated still exhibit didactic value.

For all these reasons, we choose to focus our teaching sequence on the concept of electrical interaction between the various components of the systems involved in different bonding types¹², and on the energy notion, so to highlight the common physical nature of the various kinds of bond, the continuum of bond forces and the energetic stabilization of the system that accompanies the spontaneous formation of any bond. In no case have we deemed it appropriate to rely on the concept of orbital or of electron as a wave, with the consequent description of the bond as a figure of interference between wave functions. On the other hand, we felt that we could not completely exclude the use of concepts borrowed from the quantum world, due to the need to refer to the atomic structure. We therefore used the Bohr shell atomic model, in which the atom is described as a system characterized by a positively charged nucleus and electrons orbiting around it, on stationary orbits characterized by specific energy values. It is a didactic choice made for high school students, i.e. the school level to which the sequence is addressed.

- ✓ **Emphasis on the aspects of continuity between different kinds of bond:** we choose to stress the common electrical origin of different kinds of bonding (Dhindsa and Treagust, 2014). In this way, we intend to avoid promoting the usual dichotomies between intra- and inter-molecular bonds, or between the covalent and ionic bonding models, denounced as a problem by didactic research. Consequently, contrary to what happens in common textbooks, our sequence follows a logical path that alternates various types of intra- and inter-molecular bonding models, by emphasizing their common nature of electrical interaction and differentiating them based on the energetic scale, i.e. the stability of the systems that are gradually taken into consideration. The sequence starts from the concept of the physical state of monoatomic substances, in which the only interactions involved are London dispersion forces. Thus the concept of instantaneous dipole is elaborated. A homologous series of simple diatomic substances is then taken into consideration: this allows highlighting the need to distinguish between interactions that occur *between* molecules and interactions present *inside* molecules¹³.

The discussion of the covalent bond (pure and polar) is followed by the construction of the concept of bond and molecular dipole. The ionic bond model emerges as a critique of the covalent bond model. Similarly, the metallic bond model is built after verifying the ineffectiveness of previously constructed models in justifying the properties of metallic substances. The discussion of the energetic aspects goes along this path.

- ✓ **Use of worksheets and problem situations:** the sequence is a logical chain of activities, each one characterized by specific learning objectives, that are consequent to the previous activities and preparatory to the following ones. The teaching action exploits practical activities, discussions in the classroom, worksheets (WS). The WSs submitted to students present experimental data, descriptions of phenomena or representations of models. Students are invited to examine data, to compare results and to reflect on the representations provided in the WS; they are asked specific questions, whose answers lead students to apply their previously acquired knowledge and/or formulate coherent

¹² We'd like to stress that this does not mean to rescue Berzelius' theories on chemical bonding. It is rather matter of reasoning on a model of atomic structure where various charged particles (electrons, protons) interact mutually. It is not even matter of denying the limits of this model: yet, the limits of Lewis' model have not prevented its author from developing it or even modern chemists from using it successfully, albeit with all the necessary caveats. Once again, it is matter of clarifying what a model is, which relationship exists between model and reality, what is the field of existence of the model and therefore which are its limits.

¹³ A primitive concept of a molecule, as an ordered aggregate of atoms, has already been constructed by students in previous activities on chemical transformations.

hypotheses. Face to a problem-situation, they are called to make choices and justify them. This favors the development of critical thinking and meta cognition, that is, the awareness of one's own learning mechanisms (Talanquer, V. 2013). The sequence WSs are projected on the LIM and the students answer in their notebook, possibly accessing the WS using their mobile phone (therefore photocopies are not necessary). The compilation (individually or in small groups) of the WS is followed by moments of discussion and sharing of the conclusions, under the guidance of the teacher. All these activities allow students to change their initial conceptions, according to a process of progressive conceptual maturation, and to develop skills.

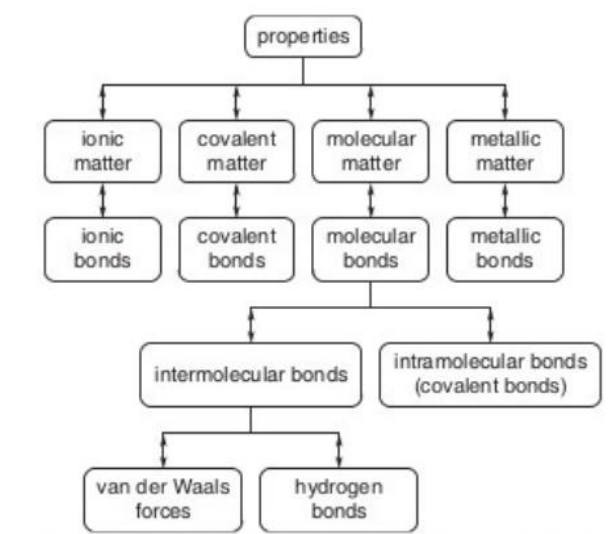
- ✓ **Use of ICT:** digital tools such as simulations and videos, are used at some points in the sequence. These tools were screened to avoid inconsistent representations of the microscopic world, that would foster misconceptions.
- ✓ **Interdisciplinarity with physics:** the physical bases of the concept of interatomic bonding make the collaboration between physics and chemistry teachers essential for developing this topic. Since this sequence relies on the concept of electrical interaction, the participation of the physics teacher is essential for building up and clarifying the notions of electric charge, electric field, electric dipole and energy.

Our teaching sequence on interatomic bonding is organized in the following sections, each with specific teaching and learning objectives:

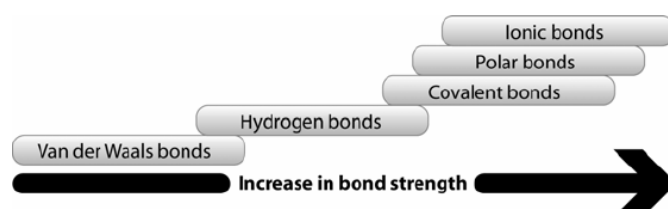
1. DETECTION OF STUDENTS INITIAL CONCEPTIONS AND PRELIMINARY ACTIVITIES
2. LONDON DISPERSION FORCES
3. COVALENT BONDING MODEL
4. DIPOLE-DIPOLE BONDING AND HYDROGEN BRIDGE BONDING
5. IONIC BONDING MODEL
6. METALLIC BONDING MODEL
7. CONCLUSIVE SUMMARY ACTIVITY

This path clearly differs from the traditional approach to chemical and intermolecular bonding, summarized in scheme A. It rather aims at emphasizing the continuum of bonding forces (Scheme B), according to Nahum et al. (2008).

A- A schematic representation of the traditional approach for teaching the chemical bonding (Nahum et al. 2008)



B- A schematic representation of the continuous scale of bond strengths (Nahum et al. 2008)



4.1 Detection of students' initial conceptions and preliminary activities

Given the role played by students' initial conceptions on the learning process, we believe essential to us to open the educational path with an activity that allows checking the students' conceptions on interatomic bonding. For this purpose, the questionnaire shown in the attached is administered to the students.

Various scholars suggest using diagnostic tools such as brainstorming (Bergqvist et al., 2016), interviews or multiple choice tests (Ünal et al. 2006), which allow the student to choose one or more answers from various possible options, either correct or incorrect.

The test we designed (Appendix A) makes use of the following types of questions:

- multiple choice with justification of the choice;
- true or false with justification of the choice;
- short answer at open questions;
- open questions that require the particle representation of a system.

The topics under investigation relate to the knowledge considered fundamental to the treatment of the chemical bond:

- the particle model;
- the concepts of atom, molecule, simple substance and compound, mixtures;
- macroscopic and microscopic properties of matter;
- the atomic shell model;
- the changes of physical states.

Learning the particle nature of matter and the relationships between the particle and macroscopic level is a necessary requirement for understanding interatomic bonding. It is advisable to deal with bonding after making sure that students are familiar with the particle description of matter and its implications. Indeed, the relationship between students' misconceptions on the particle nature of matter and those on the interatomic bonding is well documented (Othman et al., 2008).

The results of the test allow the teacher to evaluate the need to re-discuss those contents that have not been effectively learnt by the students.

This first activity is followed by the examination of the macroscopic properties of a group of substances, assigned by the teacher to the class. Students are asked to compile a table collecting physical data of various materials, and behaviours such as their solubility/miscibility in water, conductivity, and fragility, obtainable from laboratory test or from data searches. The expected result is summarized in Table 4.1.

Table 4.1

Material	Physical state at room P and T	Density at 20 °C (g/cm3)	Melting point (°C)	Solubility in water	Conductivity at room T and P	Conductivity in water	Conductivity in the liquid state	Fragility
Sodium chloride	Solid	2,16	801	Soluble	Non-conducting (solid state)	Conductor	Conductor	Fragile
Copper	Solid	8,9	1084,6	Insoluble	Conductor (solid state)	= =	Conductor	Not fragile
Iron	Solid	7,86	1535	Insoluble	Conductor (solid state)	= =	Conductor	Not fragile
Gold	Solid	19,3	1064	Insoluble	Conductor (solid state)	= =	Conductor	Not fragile
Quartz	Solid	2,65	> 2000	Insoluble	Non-conducting (solid state)	= =	Non-conducting	Fragile
PET (plastic)	Solid	1,3-1,4	245-265	Insoluble	Non-conducting (solid state)	= =	Non-conducting	Not fragile
Sucrose	Solid	1,59	186	Soluble	Non-conducting (solid state)	Non-conducting	Non-conducting	Fragile
Diiodine	Solid	4,9	113,7	Slightly soluble	Non-conducting (solid state)	= =	Non-conducting	Fragile
Sulfur	Solid	2,07	113	Insoluble	Non-conducting (solid state)	= =	Non-conducting	Fragile
Ethanol	Liquid	0,79	-114	Soluble	Non-conducting (liquid state)	Non-conducting	Non-conducting	= =
Dioxygen	Gas	0,00143 (P = 1 atm)	-218,8	Soluble	Non-conducting (gaseous state)	Non-conducting	Non-conducting	= =

The goal of this activity is to highlight the variety of behaviors and properties of materials and substances. Students, through previous activities on physical and chemical transformations, have already acquired the habit of formulating microscopic interpretations (modeling) of phenomena observed at the macroscopic level. The class discussion therefore aims at highlighting the wide range of properties exhibited by substances and to stimulate the search for explanatory models.

Students will get back to this table during the teaching sequence.

Once the table completed, the teacher will stimulate the discussion in the classroom through questions such as:

- Do you think possible to group substances/materials into homogeneous groups based on their properties?
- Based on what you have learnt so far, how do you justify the existence of such marked differences between one type of substance/material and another?

As the first step, students will identify empirical classification criteria and build sets of substances, based on their properties. These sets will be generically named A, B, C etc. The classification of substances as ionic, metallic, etc. – that many textbook present as introductory steps to the topic of interatomic bonding (Nahum et al. 2008) – will be achieved only after learning various bonding models. This choice is aimed at helping students understand the meaning of such classifications and the fact that they derive from the application of distinct bonding models.

So, students are expected to identify the following sets:

SET OF SUBSTANCE	EXAMPLE	CHARACTERISTICS
A	Sodium chloride	Solids at room T and P Non-conducting at solid state Conductor in solution Soluble in water High melting points Fragile
B	Copper Iron Gold	Solids at room T and P Conductor in solid state Insoluble in water High melting points (although, quite variable from one substance to another) Not fragile
C	Quartz Sucrose Diiodine Sulfur Ethanol Dioxygen	Various physical states at room T and P Not-conducting at solid state Soluble or insoluble in water Not-conducting in solution Very variable melting points Fragile
D	PET	Solids at room T and P Not-conducting at solid state Non soluble in water Relatively low melting points Not fragile

The students, to whom this sequence is proposed, have learned the particle model of matter and they are used to applying it to interpret simple phenomena relating to the material world: that is, they are used to correlate macroscopic evidence with microscopic interpretations. The second question posed by the teacher aims at stimulating the search for microscopic models that allow interpreting the variety of properties highlighted here.

4.2 *London dispersion forces*

This segment of the sequence focuses on the London dispersion forces. The choice to address this issue as a priority is based on various reasons. First, the London dispersion forces affect all types of chemical species and thus represent the most general type of interatomic interaction. Second, by tackling them first, it is possible to discuss monatomic substances that avoid the conceptual complications related to molecular systems, where intra- and inter-molecular bonds coexist. In fact, several researches (Cokelez et al. 2008) highlight the difficulty of many students in distinguishing the two types of bond and in understanding which of the two is involved in the chemical and physical transformations of matter. The learning objectives of this segment are:

- to understand that London dispersion forces are generated by the presence of temporary dipoles;
- to understand that these dipoles are generated by the charge interactions between nucleus and electrons and, more in details, by the endless motion of electrons around nuclei;
- to understand that, despite the low energy involved, these interactions may be responsible for the formation of condensed states (liquid and solid state).

To achieve these learning objectives, problem situations are used concerning the trend of melting and boiling temperatures of noble gases (monatomic systems or mononuclear molecules, according to the terminology suggested by Jensen 1998). The literature reports various examples of activities where the trend of melting and boiling temperatures of substances is correlated with their microscopic structure (Melinda Ogden, 2017; Schmidt et al., 2009) so to promote the understanding of intermolecular forces. As for the preparatory knowledge and skills for these activities: students already know how to model physical states at the microscopic level (through the particle model of matter) and to represent them iconographically according to this model. Further, they have already learned the distinction between chemical transformation and physical transformation.

A terminological remark: in the first worksheets of the sequence, we distinguish between interaction and constraint. Interaction is any form of energy exchange between particles; constraint is an interaction that limits the translational freedom of particles, preventing them from moving away at an infinite distance. In this first phase we avoid introducing the term *bond* and we use the term *constraint* instead. Only after the students have realized that these constraints are due to the existence of attractions and repulsions of electrical nature, the term *bond* will be introduced: it will then be conceptually meaningful.

Activity 1

The objective of this activity is to lead students to the idea that the formation of a condensed physical state involves the presence of constraints between the components of the system and that such constraints also exist in a substance such as helium, which can exist at liquid and solid state only at very low T and high P. The macroscopic data available to students are the values of the melting and boiling temperatures of the simple substance He. Students are therefore required to represent the three physical states of helium at the microscopic level (atomic/molecular) justifying what they have done and to explain if and in which cases they believe there are constraints between the particles.

Object of the proposed activity	Learning objectives
Students are asked to represent He in the solid state, in the liquid state and in the gaseous state by using the particle model, and to reflect on the presence or absence of constraints between the atoms in the three cases.	To consolidate the concept that the condensed state of a substance is always associated with the existence of constraints between the structural units of that substance.

The simple substance Helium (He) has a melting point of 0.95 K ($p = 2.5$ MPa) and a boiling point of 4.22 K.

1. Represent the simple substance He in the solid state, in the liquid state and in the gaseous state, at the atomic/molecular microscopic level:

2. Do you think that among the atoms of the solid simple substance He:
 - there are no constraints;
 - there are constraints;
 - it is not possible to answer;
 - I can't answer.

Justify your choice:

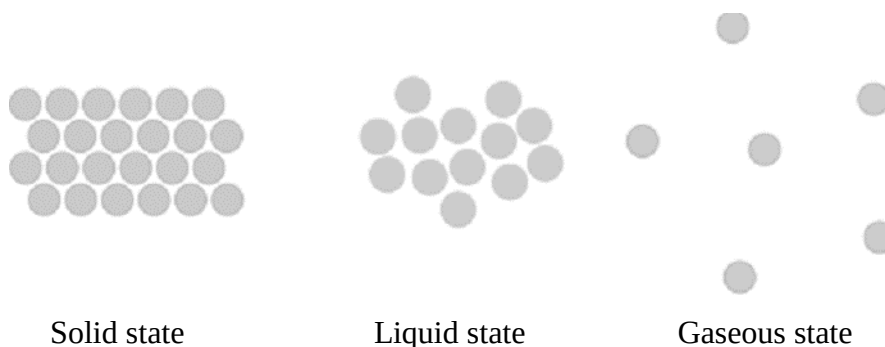
3. Do you think that among the atoms of the liquid simple substance He:
 - there are no constraints;
 - there are constraints;
 - it is not possible to answer;
 - I can't answer.

Justify your choice:

4. Do you think that among the atoms of the gaseous simple substance He:
 - there are no constraints;
 - there are constraints;
 - it is not possible to answer;
 - I can't answer.

Justify your choice:

The teacher, after leaving students enough time to carry out the assignments of point 1, engages students in a discussion on question 1 with. The aim is to lead student to share the following microscopic representations of the simple substance He in the solid, liquid and gaseous physical state:



The discussion extends to questions 2, 3 and 4. The teacher leads the classroom towards the following conclusion: **in solid and liquid states, the particles are close to each other and they are constrained; in the gaseous state, the particles are far away from each other and there are no constraints between them.** The weakness of the interaction between He particles is witnessed by the need to apply considerable pressure to obtain the solid state (as lowering T is insufficient).

Activity 2

Goal of this activity is to highlight the correlation between melting and boiling temperatures of a substance and the entity of the constraints between particles. For this purpose, the physical data of two monoatomic substances (He and Ne) are compared.

Object of the proposed activity	Learning objectives
The melting and boiling temperatures of the simple substances He and Ne are compared; the entity of the constraints between He and Ne particles are discussed.	To understand the correlation between the values of melting and boiling temperatures of a substance and the entity of the constraints between the structural units of that substance

WS 2

The simple substance Helium (He) has a melting point of 0.95 K ($p = 2.5$ MPa) and a boiling point of 4.22 K. The simple substance Neon (Ne) has a melting point of 24,56 K and a boiling point of 27.07 K.

Based on these pieces of information, do you think that:

- the constraints between He atoms are stronger than those between Ne atoms;
- the constraints between Ne atoms are stronger than those between He atoms;
- it is not possible to answer;
- I can't answer.

Justify your choice:

The discussion carried out in the classroom aims at getting to the following conclusion: **since Neon's melting and boiling temperatures higher than Helium's, the entity of the constraints between Ne atoms is greater as compared to He atoms. Melting and boiling temperatures are proportional to the entity of interparticle interactions.**

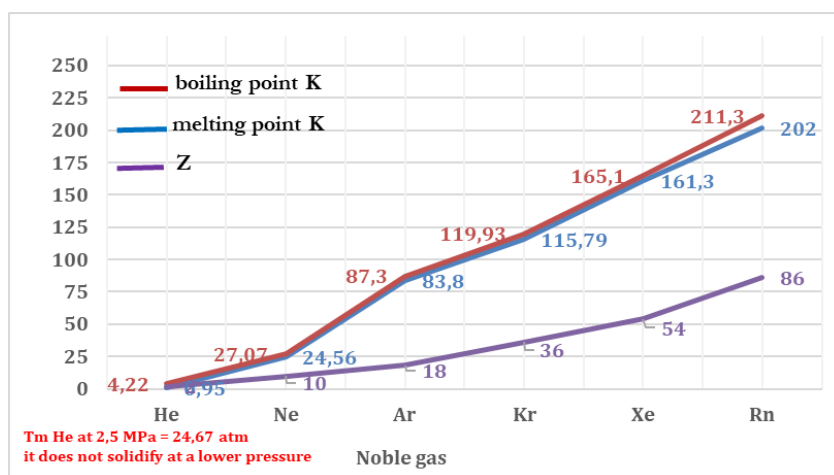
Activity 3

The purpose of activity 3 is to consolidate the learning objective of WS 2, by extending the comparison to multiple substances belonging to a homologous series. Students are provided with the melting and boiling temperatures of all noble gases and are asked to order these substances according to the increasing entity of the constraints between their particles.

WS 3

Examine the melting and boiling temperatures of noble gases shown in the following table and in the following graph:

Noble gas	Melting temperature	Boiling temperature
He	0,95	4,22
Ne	24,56	27,07
Ar	83,8	87,3
Kr	115,79	119,93
Xe	161,3	165,1
Rn	202	211,3



Based on these pieces of information, order the noble gases according to the increasing extent of the constraints existing between their particles. Justify your answer:

The results are discussed in the classroom. The teacher summarizes the conclusion: **the melting and boiling temperatures of noble gases increase in the following order He, Ne, Ar, Kr, Xe and Rn; the entity of the**

constraints between atoms of each noble gas grows in the same order. The teacher will point out that the trend of melting and boiling temperatures correlates with the increase in atomic numbers, that is the number of electrons in each atom of gas. This observation is relevant as - at a later stage - students be ask to think about the number of electron in each atom of a substance and the entity of the interaction between temporary dipoles. These first three activities aim to highlight the dependence of the melting and boiling temperatures (macroscopic properties) on the entity of the constraints between particles of a substance (microscopic properties).

Activity 4

At this point, students are asked to investigate the material cause of the constraints between particles, which were previously discussed. Constraints originate from electrical interactions; therefore, it is necessary to lead students to think about attractions and repulsions between electrical charges, and what determined their entities. Since electrostatic interactions are governed by *Coulomb's law*, WS 4 aims at making student understand the meaning of its mathematical expression. Coulomb's law should have already been studied in the physics course. This activity exploits a simulation that helps students verifying the qualitative and quantitative application of the "*Coulomb's law*" (<https://phet.colorado.edu/it/simulation/coulombs-law>). WS 4 helps student to use this application effectively: it contains questions on the effect of the sign, the extent and the distance between charges.

Object of the proposed activity	Learning objectives
A simulation is used which allows verifying Coulomb's law in its qualitative and quantitative aspects.	To check Coulomb's law and to understand its physical meaning.

Try the following simulation: <https://phet.colorado.edu/it/simulation/coulombs-law>

Set the value of the two electric charges, **one positive and one negative**, at your choice and keep their distance unchanged.

1. The interaction between the two charges is:
 - repulsive;
 - attractive;
 - it is not possible to answer;
 - I can't answer.

2. When one or both electric charges are increased, how does the extent of the interaction between the two charges vary?
 - it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.

Set the value of the two electric charges, **one positive and one negative**, at your choice and change their distance.

3. If the distance between the two charges increases, how does the extent of the interaction between the two charges vary?
 - it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.

4. If the distance between the two charges decreases, how does the extent of the interaction between the two charges vary?
 - it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.

Set the value of the two electric charges, **both positive**, at your choice and keep their distance unchanged.

5. The interaction between the two charges is:
 - repulsive;
 - attractive;
 - it is not possible to answer;
 - I can't answer.

6. When one or both electric charges are increased, how does the extent of the interaction between the two charges vary?
- it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.

Set the value of the two electric charges, **both positive**, at your choice and change their distance:

7. If the distance between the two charges decreases, how does the extent of the interaction between the two charges vary?
- it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.
8. If the distance between the two charges decreases, how does the extent of the interaction between the two charges vary?
- it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.

Set the value of the two electric charges, **both negative**, at your choice and keep their distance unchanged:

9. The interaction between the two charges is:
- repulsive;
 - attractive;
 - it is not possible to answer;
 - I can't answer.
10. If the electric charge of a single charge or both increases, how does the extent of the interaction between the two charges vary?
- it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.

Set the value of the two electric charges, **both negative** at your choice and change their distance:

11. If the distance between the two charges increases, how does the entity of the interaction between the two charges vary?
- it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.
12. If the distance between the two charges decreases, how does the extent of the interaction between the two charges vary?
- it does not vary;
 - it decreases;
 - it increases;
 - it is not possible to answer.

Once this activity has been carried out by students, the teacher opens the discussion. He aims at summarising some basic principles: **i) charges of the same sign repel each other, whereas charges of opposite sign attract each other; ii) the extent of the attractive or repulsive force, at a given interparticle distance, increases with the absolute value of charges and viceversa; iii) the magnitude of the attractive or repulsive force between two given charges increases when the distance between the charges decreases and viceversa.** After sharing the previous concepts, the teacher recalls the mathematical expression of *Coulomb's law*:

$$F = k \cdot (|q_1 \cdot q_2|/d^2)$$

The dependence of the electric force F on the absolute value of charges q and their distance d can be verified through numerical examples. This highlights that the charge attractions and repulsions are “short range” forces, as their extent is only relevant when d is small.

Activity 5

Understanding the mechanism by which London dispersion forces are generated and act, requires students to understand that electrons are charged particles in endless motion. This leads to non-symmetrical charge distributions, instant by instant. These asymmetrical charge distribution is represented through symbols δ^+ and δ^- . These symbols are often misinterpreted by students.

It is relevant to understand that they do not designate “small” positive and negative charges: instead, they are a way of representing the effects of the unceasing change of charge distribution determined by electron mobility. δ^+ and δ^- designate charge accumulation or deficiency as compared to the ideal and static situation of symmetrical charge distribution within a system. In other words, δ^+ and δ^- designate situations in which the barycenters of positive and negative charges within a chemical species do not coincide.

The concerned species keeps electrically neutral, despite the asymmetric charge distribution indicated by δ^+ and δ^- ; in fact, the overall extent of negative charge keeps unchanged in the system and counterbalances the nuclear positive charge. The interpretive key of the phenomenon designated as 'London dispersion forces' is therefore the electrons' mobility around the atomic nucleus. A challenge of WS5 is make sure that students do not take symbols δ^+ and δ^- - that designate an asymmetric charge distribution - as the representation of net electrical charges (which are represented by + and - signs). In order to achieve this goal, we propose using a video, that helps consolidating the idea of the endless movement of electrons: students are then invited to represent a Helium atom in single static moments (like movie's frames). The comparison between several successive situations leads to understand that - although the atom remains neutral because the sum of the positive and negative charges does not vary - however the barycenter of negative charges does not always coincide with that of positive charges. This happens because the movement of the electrons determines instantaneous asymmetric distributions of the negative charge. Whenever this occurs, we say that a dipole has been generated. This activity has a high interdisciplinary content, as it provides the opportunity to integrate the teachings of chemistry and physics, as required by the subject "Integrated Sciences" (found in Italian high schools). In the physics course, the concept of electric dipole is usually introduced at the second grade, within the electrostatics module, to justify the polarization of insulating materials (dielectrics) in the presence of an external electric field. The (macroscopic) phenomenon is interpreted at the microscopic level, precisely in terms of asymmetric charge distribution of the particles in the dielectric. The knowledge deriving from the study of electrostatics should therefore facilitate the construction of the dipole concept at the microscopic level.

Object of the proposed activity	Learning objectives
An animation is proposed that highlights the motion of electrons around the atomic nucleus	To consolidate the concept of electron mobility
Students are asked to represent a Helium atom at the nuclear-electronic level in successive instants, and to compare their representations	To build the notion of barycenter of negative and positive charges within an atom.
	To build the concept of atomic dipole as a situation where the barycenters of positive and negative charges do not coincide. To build the concept of instantaneous dipole as a consequence of electron mobility.

Look at the following animation which refers to an atomic nucleus surrounded by its own electrons:
<https://it.depositphotos.com/13705713/stock-video-atom-loop.html>

1. Represents a Helium atom at the nuclear-electronic level at the hypothetical instant 1 (one):

Justify your representation:

2. Represents a Helium atom at the hypothetical instant 2 (two) that follows instant 1 (one):

Justify your representation:

3. Do you think the electrons occupies the same position at instant 1 and instant 2?

- yes; I do;
- no, I don't;
- it is not possible to answer;
- I can't answer.

Justify your answer:

4. How do you believe that negative and positive charges are distributed within the atom at instants 1 and 2:

- symmetrically;
- asymmetrically;
- it is not possible to answer;
- I can't answer.

Justify your answer:

5. Do you think that at instants 1 and 2 the Helium atom is:

- neutral;
- positively charged;
- negatively charged;
- it is not possible to answer.

Justify your answer:

6. Do you think that at instants 1 and 2 the barycenters of the positive and negative charges in the Helium atom coincide?

- yes, I do;
- no, I don't;
- it is not possible to answer;
- I can't answer.

Justify your answer:

7. Look at the following representation:



How do you believe that negative and positive charges are distributed within the atom:

- symmetrically;
- asymmetrically;
- it is not possible to answer;
- I can't answer.

Justify your answer:

8. Do you think that in the previous representation the Helium atom is:

- neutral;
- positively charged;
- negatively charged;
- it is not possible to answer.

Justify your answer:

9. Do you think that in the previous representation the barycenters of the positive and negative charges in the Helium atom coincide?

- yes, I do;
- no, I don't;
- it is not possible to answer;
- I can't answer.

Justify your answer:

10. We have considered that electrons move endlessly around the atomic nucleus, changing their position instant by instant. In the light of this consideration, do you believe that the barycenter of the positive and negative charges in an atom always coincide, instant by instant?

- yes, I do;
- no, I don't;
- it is not possible to answer;
- I can't answer.

Justify your answer:

11. During the physics lessons, we learnt that when the barycenters of the negative and positive charges do not coincide in a system, we have an electric dipole. The video we watched shows that electrons move continuously around the atomic nucleus, changing their position instant by instant. In the light of these considerations, you believe that the Helium atom is:

- always an electric dipole;
- never an electric dipole;
- an electric dipole that varies from moment to moment;
- I can't answer.

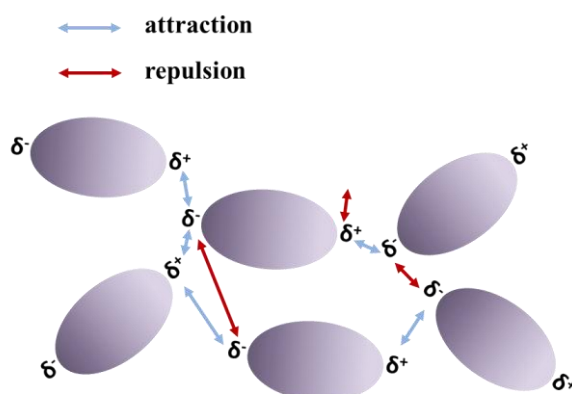
Justify your answer:

The achievement of the learning objectives of this activity should be facilitated by the activities on electrical dipoles addressed in the Integrated Sciences-Physics course.

Regarding WS 5, we observe that:

- In the representations required by questions 1 and 2 students are expected to indicate asymmetric distributions of electrons around the nucleus, as these are the most probable. Should they draw at least one symmetrical representation, the questions are formulated in a way that allows the comparison between symmetrical and asymmetrical situations.
- Questions 4, 6, 7, and 9 aim at making students understand that, due to the mobility of electrons, the barycenter of negative charge changes instant by instant.
- Questions 5 and 8 aim at making clear that the change of charge distribution in space does not affect the total net charge of the atom, which remains unchanged and equal to zero.
- Questions 10 and 11 aim at making clear that a dipole always corresponds to a situation in which the barycentres of positive and negative charges of the system do not coincide; in addition, the electrons' motion can generate temporary dipoles.

The teacher highlights the temporariness of electric dipoles and discusses their role in generating those constraints between particles that are responsible for the formation of condensed states (solid and liquid state), as discussed in previous activities. The teacher proposes a representation of the interactions between dipoles (see below) and underlines the continuous variability of this distribution:



Furthermore, the teacher introduces the symbology δ^+ and δ^- and discusses its meaning in the light of the concepts built with WS 5: any asymmetrical charge distribution in space (and time) is represented with symbols δ^+ and δ^- . They do not designate small electrical charges, they rather report the asymmetry of electrons' distribution, that varies instantaneously due to the mobility of electrons.

At this point it is possible to replace the term *constraint* (previously employed) with the term *bond*, as students have clarified its nature (of electrical interaction) and its origin (due to electronic mobility). The teacher will conclude the discussion by defining **the bonds called London dispersion forces as those electrical interactions that are formed between temporary dipoles and are responsables for the interactions between noble gas atoms.**

Activity 6

Once the nature and origin of the London dispersion forces have been clarified, it is appropriate to introduce quantitative elements. The purpose of WS 6 is to allow students to link the nature of the constraints between particles (highlighted in WS 1) to the London dispersion forces and to link the entity of these constraints between particles (WS 2 and 3) to the number of electrons found in atoms of noble gases. Students are required

to represent substances He and Ne in the solid state at the nucleus/electron microscopic level, as the description of interatomic bonds requires treatment at this level of representation. This allows students to relate the number of electrons in each atom with the entity of the London forces between atoms and to understand that these forces act only at short distances between particles: in fact, only in solid and liquid states temporary dipoles are sufficiently close to generate constraints. In the gaseous state, dipoles are too far apart and the interactions between them are so weak that there are no constraints.

Object of the proposed activity	Learning objectives
Students are asked to represent He and Ne substances in the solid state at the nucleus/electron microscopic level.	To understand that the constraints between the He and Ne atoms arise from the formation of temporary dipoles.
The different bond strengths between atoms of noble gases are compared.	To correlate the extent of these constraints between atoms of noble gases with the number of electrons found in each atom

WS 6

1. Represent the simple substances He and Ne in the solid state at the nuclear-electronic level

2. How do you explain the existence of constraints between He atoms and between Ne atoms?

3. How do you explain the trend of the extents of the constraints between He, Ne, Ar, Kr, Xe and Rn atoms that was hypothesized in WS 3?

Question 2 connects to WS 5: the representations of He and Ne at the nuclear-electronic level in the solid state should lead students to realize that, instant by instant, these atoms are characterised by an asymmetric distribution of negative charges. Consequently, an instantaneous electric dipole is associated with each atom and individual dipoles undergo mutual electric attractions, which have been called *London dispersion forces* and bind noble gas atoms together. The comparison of the representations of He and Ne (that has more electrons than Helium) and the observation that the extent of interatomic constraints is greater in Ne as compared to He aims at highlighting the connection between the extent of these constraints and the number of electrons in each atom. This correlation is confirmed by the comparison with the other noble gases, already mentioned in WS 3.

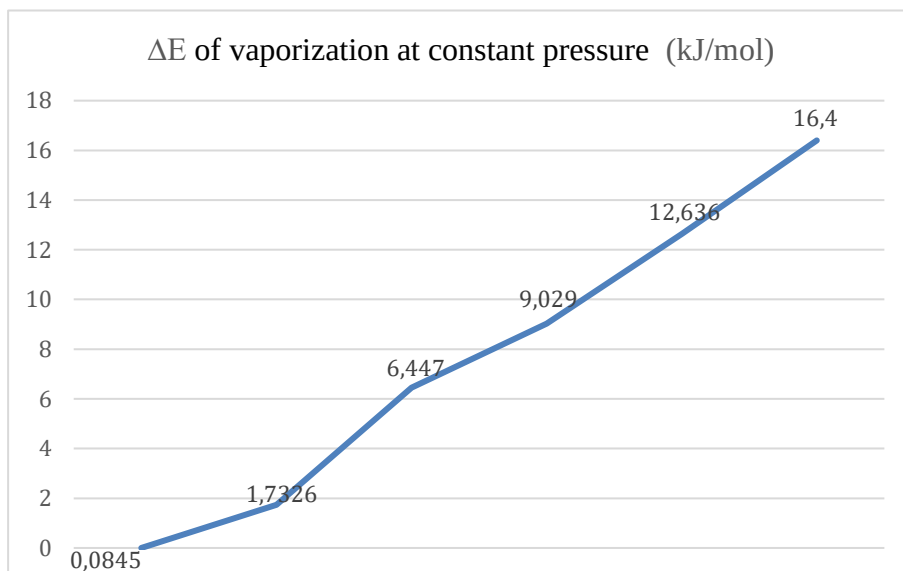
The shared conclusion is that **the extent of those bonds called *London dispersion forces* increases with the number of electrons (that is, the atomic number).**

Activity 7

Here the concept of bonding energy is introduced. To this purpose, vaporization enthalpy values are used: in fact, vaporization implies shifting from a physical state wherein particles are constrained to another wherein particle are freely moving in space. Vaporization enthalpy is defined as the energy required to vaporize a mole of substance at its boiling point, at standard pressure. In the IS, the vaporization enthalpy is expressed in kJ/mol. In WS 7, students are asked to associate each noble gas with the correct vaporization energy value at constant pressure and to justify their choice. We prefer to use the term *energy* instead of *enthalpy*, which may not be familiar to students and which will be dealt with in later school grades. Subsequently, they are asked for a definition of bonding energy which is closely related to the amount of vaporization energy.

Object of the proposed activity	Learning objectives
The graph of the vaporization energies at constant pressure of the noble gases is analyzed	To understand that the extent of vaporization energy at constant P is related to the extent of London dispersion forces
Students are requested to propose a definition of bonding energy	To understand that the extent of vaporization energy at constant P is related to the bonding energy between noble gas atoms.

1. Look at the graph reporting the vaporization energies of noble gases. Vaporization energies are the energies required to vaporize a mole of substance at its boiling temperature, at standard pressure. Based on your knowledge of noble gases, associate each noble gas with its corresponding vaporization energy. Write the symbols of the noble gases on the abscissa at each energy value.



2. Explain the criteria you followed in making your assignments

3. Propose a definition of bonding energy:

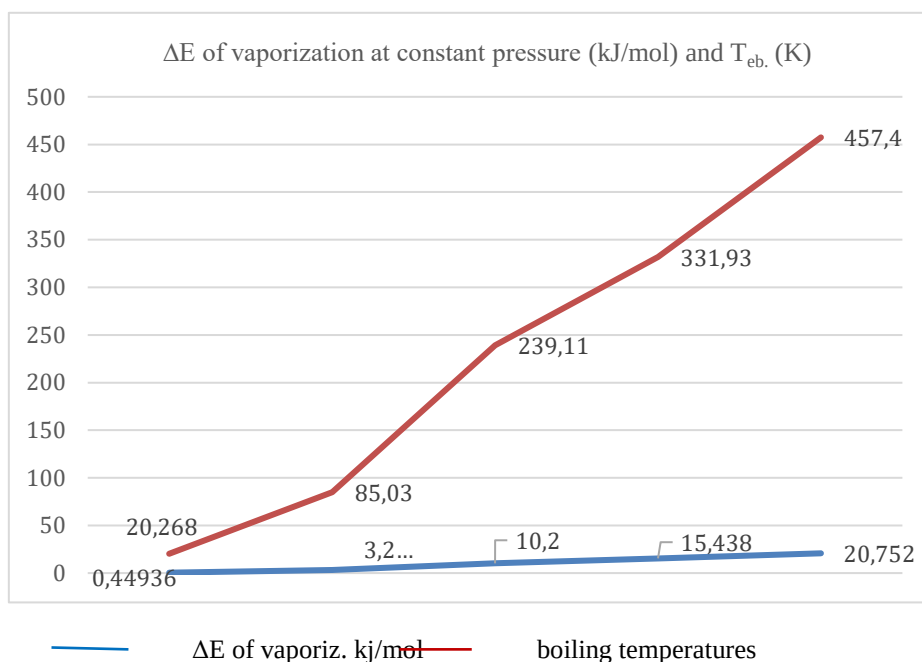
The results of the individual activity are shared with the classroom and discussed under the teacher's guide. It is pointed out that vaporization energy values grow along the homologous series of Noble gases: **vaporization energy values increase with the extent of London dispersion forces and with Z**. The trend of the graph in WS 7 is similar to the trend of melting and boiling temperatures (see previous activities). This means a greater amount of energy is required to break/weaken interparticles interactions and induce the liquid-gas state transition, as Z increases. After discussion, a shared definition of bonding energy is proposed: it is **the amount of energy required (i.e. to be supplied to the system) to break or weaken interatomic bonds**. As a result, students are led to realize that the same amount of energy *is released* by the system whenever bonds are formed. Hence, bonding energy is a measure of the system's stabilisation.

Activity 8

The goal of this activity is to consolidate the understanding of the correlation between the extent of the London dispersion forces and the total number of electrons found in the constituent particles of a substance. The same type of activity as WS 7 is therefore proposed, but it refers to a new homologous series of simple substances: H_2 , F_2 , Cl_2 , Br_2 , I_2 .

WS 8

1. Look at the graph of the boiling temperatures and vaporization energies of simple substances H_2 , F_2 , Cl_2 , Br_2 , I_2 . Associate each simple substance with its corresponding boiling temperature and vaporization energy. Write the symbols of the substances along the abscissa, at each energy value.



2. Explain the criteria you followed in making your assignments

In WS 8, students must apply their previous knowledge to a new homologous series of simple substances. They are expected to easily get to the conclusion that:

- **in a homologous series of substances, as the number of electrons increases, the extent of the London dispersion forces increases. This is signaled by the increase in boiling temperatures and vaporization energies at constant P.**

Activity 9

The purpose of this WS is to bring out the **difference between intermolecular and intramolecular bonds**: this will lead students to mobilize their previously acquired knowledge on the distinction between chemical and physical transformations and to locate it into a more detailed frame. They are required to draw the iconic representations of the diatomic substance H_2 in the different physical states at the atomic-molecular level, so to highlight that state transitions affect only bonds between the H_2 molecules (i.e. the London dispersion forces), without perturbing the H_2 entity (i.e. bonds inside H_2). This is proven by the fact that substance H_2 persists during the transformation: only its state of aggregation changes.

Object of the proposed activity	Learning objectives
Students are required to represent the diatomic substance H_2 in different physical states by means of representations at the atomic-molecular microscopic level.	To identify that the system is characterised by two distinct types of bonds; to recall the fact that physical transformations affect only one of the two types of bonds, the inter-molecular one.

The simple substance H_2 has a melting point of 14.025 K and a boiling point of 20.268 K

1. Represent the simple substance dihydrogen in the solid, liquid and gaseous state from the atomic-molecular microscopic point of view.

Justify your representations:

2. Do you think that the simple substance dihydrogen transforms into another substance during fusion?
 - Yes, I do;
 - No, I don't;
 - it is not possible to answer;
 - I can't answer.

Justify your answer:

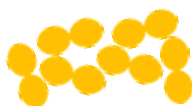
3. Do you think that the simple substance dihydrogen transforms into another substance during vaporization?
 - yes I do;
 - No, I don't;
 - it is not possible to answer;
 - I can't answer.

Justify your answer:

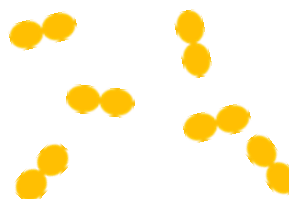
During the discussion in the classroom, students comment microscopic representations of the simple substance H_2 in the three physical states solid, liquid and gaseous, like the following ones:



H_2 in the solid state



H_2 in the liquid state



H_2 in the gaseous state

Students are familiar with these representations because they have already used them in previous activities on the physical transformations of matter.

The teacher summarizes the outcomes of the discussion and states the following conclusion:

during the physical transformations of a substance, the change of some macroscopic features (volume, shape, compressibility) can be observed, but the substance keeps unchanged. This finding can be interpreted at the microscopic level as a consequence of the weakening of bonds between the substance' molecules. The molecule remains unchanged because the corresponding substance remains the same throughout the transformation.

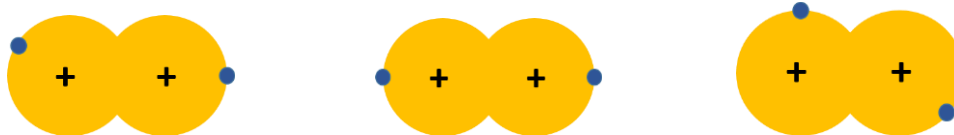
The teacher may stimulate students to discuss the reasons of the substance's persistence: students have already met the notion of molecule. They may be led to discuss about the presence of interactions between the atoms within the molecule and to compare their extent to the extent of London Forces. When interatomic bonds break/loosen easily, the interatomic interaction is weaker; conversely, if interatomic bonds are hardly broken or loosened, the interatomic interaction is stronger. This is the case of interatomic bonds inside the molecule as compared to London forces.

Activity 10

This activity aims at leading students explore the origin of interactions between H_2 molecules. In fact, the electrons within the H_2 molecule, just like those in the He atom, move endlessly around the nuclei. This implies that the barycenters of positive and negative charges may or may not coincide, instant by instant, although the molecule is electrically neutral. So in H_2 molecules, just as in Helium atom, temporary electric dipoles are generated instant by instant.

Object of the proposed activity	Learning objectives
Students are shown the representations of the dihydrogen molecule at the nuclear-electronic level in successive instants: they are invited to compare the representations with each other.	To consolidate the concept of electron mobility and to extend it to polyatomic systems.
	To consolidate the concept of dipole as a system wherein the barycenters of positive and negative charges do not coincide.
	To consolidate the concept of instantaneous dipole as a consequence of the mobility of electrons around positively charged nuclei.

Look at the following representations of the H_2 molecule at three different times:



- Do you think the position of the electrons is the same in each of the three moments?
 - yes, I do;
 - no, I don't;
 - it is not possible to answer;
 - I can't answer.

Justify your answer:

- Do you think that - in each instant represented in the previous figure - the H_2 molecule is:
 - positively charged;
 - neutral;
 - negatively charged;
 - it is not possible to answer.

Justify your answer:

- You learnt that electrons (which are negatively charged) move continuously around nuclei (which are positively charged), hence they change their position instant by instant. In the light of this consideration, do you believe that the barycenters of the positive and negative charges coincide, moment by moment, in the H_2 molecule?
 - yes, I do;
 - no, I don't;
 - it is not possible to answer;
 - I can't answer.

Justify your answer:

- You learnt that a system in which the barycenters of negative and positive charges do not coincide is an electric dipole. Conversely, whenever these two barycenter coincide, there is no electric dipole. In the light of these considerations, do you believe that the H_2 molecule is:
 - always an electric dipole;
 - never an electric dipole;
 - an electric dipole that varies moment by moment;
 - I can't answer.

Justify your answer:

This WS, built along the lines of WS 5, intends to stimulate students to establish analogies between the He system and the H₂ system in terms of symmetrical or asymmetrical charge distribution in relation to electron mobility. The discussion in the classroom and the analysis of students' answers should bring out the fact that, just like the case of Helium, the dihydrogen molecule is also characterised by electrons endlessly moving around the nuclei, which generate temporary charge distribution asymmetries, that is, instantaneous electrical dipoles.

The teacher will point out that the formation of these instantaneous dipoles at the microscopic level allows interpreting the macroscopic physical behavior of substance H₂ (states of aggregation vs. T).

The teacher asks students to draw representation of the interactions between dihydrogen molecule the dipoles, just like they did for Helium atoms.

Activity 11

After having highlighted the similarities between Helium atoms and H₂ molecules, it is now time to focus on the differences between them, in terms of the extent of London dispersion forces. These differences are to be interpreted at the nuclear-electronic level.

Students are first invited to compare the nuclear-electronic structures of the He and H₂, by highlighting similarities and differences. Then the values of vaporization energies and boiling temperatures of the two substances He and H₂ are shown to students (table WS 11): the teacher wish to highlight that these parameters are about five times greater in H₂ as compared to He. Based on the knowledge available to students, this means that the entity of the London dispersion forces between instantaneous dipoles is greater in H₂ than in He. What is the reason?

The H₂ molecule has the same number of electrons as the He atom (therefore the total negative charge is the same in both cases). The total positive charge is also the same in the two systems, but the molecule of dihydrogen has two nuclei. The difference between He and H₂ does not lie in the charge entity, but in its space distribution. Could this affect the extent of London's dispersion forces? The questions of WS 11 aim to clarify that – in dihydrogen - the positive charge is spread over two centers and the electronic charge is distributed over a space region of distinct amplitude and shape as compared to Helium. The attractive power of two H nuclei is less affective as compared to He. The combination of these factors modifies the interplay of attractions and repulsions between nuclear and electronic charges, it influences the negative charge distribution instant by instant, thus easing the formation of instantaneous dipoles. In other words, this determines a greater predisposition of the binuclear molecule to generate asymmetric charge distributions, i.e. situations in which the barycenters of the positive and negative charges do not coincide. Consequently, in H₂ the extent of London dispersion forces between instantaneous dipoles is greater than in Helium. This explains why the values of vaporization energies and boiling temperatures are greater for H₂ than for He.

Object of the proposed activity	Learning objectives
The vaporization energies and the boiling temperatures of He and H ₂ are compared in order to verify the validity of the previously established correlations between the bonding energy values and the number of electrons present in a chemical species.	To understand that the extent of London's dispersion forces depends not only on the number of electrons, but also on the number of nuclei with which they interact and on the modalities of their spatial distribution.

Look at the following representations of the constituent particles of simple substances He and H₂ from the nuclear-electronic point of view:



1. What do these two particles have in common?

2. In what are these two particles different?

Look at the table below, which shows the values of the vaporization energies and boiling temperatures of simple substances He and H₂.

	He	H ₂
ΔE_{vap} (kJ/mol)	0,0845	0,4494
T_{eb} (K)	4,22	20,27

It is easy to see that the values for dihydrogen are about five times higher than for Helium.

3. In the light of what you learnt so far, do you believe that the extent of the interactions between the substance's particles is:
- greater for He than for H₂;
 - smaller for He than for H₂;
 - it is not possible to answer;
 - I can not answer.
4. Is the trend of vaporization energies and T_{eb} in agreement or in disagreement with what you learnt so far regarding the relationship between the extent of London's interactions and the number of electrons found in the system?
- In agreement;
 - In disagreement;
 - it is not possible to answer;
 - I can not answer.

5. Is the volume wherein the electrons moves equal in the He atom and the H₂ molecule?
- equal;
 - different;
 - it is not possible to answer;
 - I can not answer.
6. In your opinion, the attraction between by He electrons and the Helium nucleus is stronger or weaker than the attraction experienced by the H₂ electrons and the two Hydrogen nuclei?
- stronger;
 - weaker;
 - it is not possible to answer;
 - I can not answer.

Justify your answer:

7. In light of your previous answers, do you think that the formation of instantaneous dipoles is easier or more difficult in the case of He as compared to H₂?
- easier;
 - more difficult;
 - it is not possible to answer;
 - I can not answer.

Justify your answer:

8. In the light of these considerations, is it possible to justify the values of vaporization energies and the boiling temperatures of the two simple substances He and H₂?
-
-

The answer to question 7 could be problematic as it requires students to understand that the way the charge is distributed (the positive charge distributed over one/two nuclei and the negative charge distributed on different volumes) influences the extent of electrical interaction.

After discussing students' answers, the class is expected to share the following conclusions:

- **the extent of London dispersion forces depends on several factors: i) the number of electrons involved; ii) their distribution in space; iii) the distribution of nuclear charges in the system.**
- **the easier instantaneous dipoles are formed, the stronger are London dispersion forces.**

Furthermore, the teacher will comment on the relationship between **the macroscopic properties of substances (e.g. vaporization energies and boiling and melting temperatures) and the substance's structure at the nuclear-electronic level.** This issue will be further discussed in relation to Van der Waals

interactions. This concludes the sequence's segment devoted to the construction of the concept of instantaneous dipole and London dispersion forces.

The examination of the homologous series of simple diatomic substances has led to the distinction between interactions *between* molecules and interactions *within* molecules. It is therefore appropriate to investigate the nature and properties of intramolecular bonding, in order to understand how it differs from the interactions between molecules. Therefore, the teacher asks the students the following question: "We have seen that both the atoms of noble gases and the hydrogen molecules interact with each other through the London dispersion forces, whose nature is electric. Noble gases are monatomic substances, whereas dihydrogen is a molecular substance. Experimental evidence tells us that it is made up of diatomic molecules. What is the nature of the bond inside the dihydrogen molecule? "

In the forthcoming WSs the pure and polar covalent bond and the Lewis model will be treated.

4.3 Covalent bonding model

This section of the teaching sequence aims at leading students to build the covalent bond model and to discriminate between pure covalent bonds and polar covalent bonds. The problem of polarity is introduced in the classical fashion, first through the *structural modeling* of diatomic molecules and then by introducing *molecular geometry* and the VSEPR theory on polyatomic molecules. The logical progression of this sequence is aimed at making clear the character of logical necessity of the conceptual tools that are gradually built up. Each conceptual acquisition is logically necessary to rationally interpret specific empirical data.

This justifies the choice of treating intra- and intermolecular interactions together, alternating them along a unitary pathway focused on the notion of electrical interaction, common to any kind of bond, regardless of its categorization. The sequential introduction of the pure covalent bond notion, Lewis structures, electronegativity and polar covalent bond notion, to finally get to the concept of molecular geometry and molecular dipole, through the VSEPR theory, are essential steps for the full understanding of all intermolecular forces. In fact, Van der Waals interactions cannot be rationalized without the notion of molecular dipole, which in turn is conceptually subordinated to the above-listed concepts. Furthermore, the construction of the notion of permanent dipole is facilitated, as it can rely on the previous work on instantaneous dipoles. Another relevant aspect of the teaching approach adopted in this sequence is the recursive treatment of many notions; in fact, by returning repeatedly to the concepts related with the bonding phenomenon, students improve their understanding and consolidate their knowledge, that becomes an integral part of their cognitive matrix.

In addition to the mechanistic aspects, energetic aspect also need to be discussed. Students are asked to compare the energies involved in different types of bonds and make deductions regarding their stability. The graph of the Lennard-Jones potential is exploited to this purpose.

Activity 12

In the previous activities, some affinities and differences between noble gases and dihydrogen have been highlighted: in both cases, it is possible to hypothesize the existence of London dispersion forces between the constituent particles of the systems; their extent is related to the values of vaporization energy. However, a fundamental difference between the two systems has been highlighted: noble gases are monoatomic, whereas dihydrogen is made up of diatomic molecules. It is therefore matter of clarifying the nature of the bond between the two hydrogen atoms and to discuss the affinities and differences between the intra- and intermolecular bonds of dihydrogen. In order to do this, a look at atomic structure is necessary (at nuclear-electronic level). This worksheet aims at discussing the (attractive and repulsive) forces acting between two hydrogen atoms that get close to each other, to form a dihydrogen molecule. The aim is to let student understand that, whenever two hydrogen atoms get close enough to each other, a number of interactions are

at play: i) electrical attractions between each nucleus and the electrons of both hydrogen atoms; ii) electrical repulsions between the two nuclei and between the electrons of each atom.

Object of the proposed activity	Learning objectives
Students are asked to represent two hydrogen atoms at the nucleus/electronic level and to identify the electrical interactions that occur when the two atoms approach each other.	To clarify the different types of interactions involved in the formation of intramolecular bonds.

In the previous activities, we represented the dihydrogen molecule, made up of two bonded/joined together hydrogen atoms, whose chemical formula is H_2 . Represents the two hydrogen atoms at the nuclear-electronic level.

Atom 1**Atom 2**

Let's think about what happens when the two atoms are very close to each other, in the light of your knowledge of the interactions between electric charges and the atomic structure.

1. In your opinion, is nucleus 1 attracted or repelled by nucleus 2 (and vice versa)?
 - Attracted
 - Repelled
 - It is not possible to answer
 - I can not answer
 2. In your opinion, does nucleus 1 attract or repel the electrons of atom 2 (and vice versa)?
 - It attracts them
 - It repels them
 - It is not possible to answer
 - I can not answer
 3. In your opinion, do the electrons of atom 1 attract or repel the electrons of atom 2 (and vice versa)?
 - They attract them
 - They repel them
 - It is not possible to answer
 - I can not answer
 4. In summary, which are the attractive and the repulsive forces at play when two Hydrogen atoms get very close to each other?
-
5. In your opinion, what prevails when two hydrogen atoms are joined to form the dihydrogen molecule?
 - the attractive forces
 - the repulsive forces
 - the attractive and repulsive forces are balanced
 - I do not know
 - it is not possible to answer

Justify your answer:

The students' answers are shared and discussed in the classroom. At the end, the teacher summarizes the following electrostatic interactions:

- Electric repulsion between electrons of atom 1 and 2

- Electric repulsion between the nuclei of atom 1 and 2
- Electric attraction between nucleus 1 and electrons of atom 2
- Electric attraction between nucleus 2 and electrons of atom 1
- Electric attraction between nucleus and electrons of the same atom

Activity 13

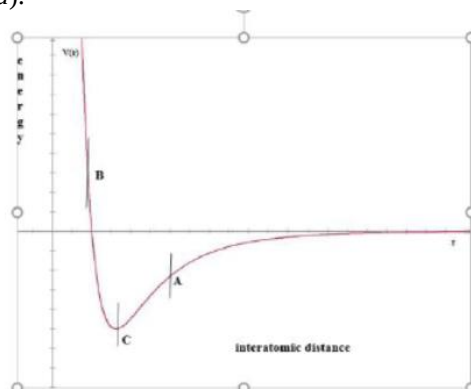
Once the presence of attractive and repulsive interactions identified, it is matter of identifying bonding as the condition where these forces are at equilibrium. This condition corresponds to a precise interatomic distance (the bond length).

It is also necessary to address energy-related aspects: the equilibrium condition minimizes the potential energy of the system and therefore corresponds to a condition of stability. To move away from this condition (i.e. weaken the bond), energy must be supplied to the system.

In WS 13 a Lennard-Jones graph is discussed: three points of this graph, corresponding to different internuclear distances are highlighted. The WS questions focus on the relationship between the relative extent of attractive and repulsive interactions at each of these three points.

Object of the proposed activity	Learning objectives
The Lennard-Jones diagram is analyzed to clarify the relationship between the extent of attractive and repulsive interactions and the bond length.	To identify the bond as an electrical interaction. To identify the bonding condition as a state of balance between attractive and repulsive interactions. Define the bond length as the average distance between the nuclei of two atoms bonded together.

Look at this graph, which shows how the energy of a system made up of 2 Hydrogen atoms depends on the distance between these two atoms: by moving from the right to left side of the abscissa, the two atoms progressively approach to each other. At the very right end they are too far from each other to interact (i.e. they are *isolated*).



1. Look at point A. In your opinion, at this point:
 - repulsive forces prevail;
 - attractive forces prevail;
 - the attractive forces and the repulsive forces are balanced;
 - I can not answer.

Justify your choice.

2. In your opinion, why does the energy decrease at point A as compared to the isolated atoms?
-

3. Look at point B. In your opinion, at this point:
 - repulsive forces prevail;
 - attractive forces prevail;
 - the attractive forces and the repulsive forces are balanced;
 - I can not answer.

Justify your choice.

4. In your opinion, why does the energy increase at point as compared to the isolated atoms?
-

5. Look at point C. In your opinion, at this point:
 - repulsive forces prevail;
 - attractive forces prevail;
 - the attractive forces and the repulsive forces are balanced;
 - I can not answer.

Justify your choice.

At the end of the classroom discussion, the teacher summarizes the conclusions: students are expected to recognize that attractive interactions prevail at point A; at point B the repulsive interactions prevail and at point C they are balanced. Furthermore, the energy decrease implies a stabilization of the system. The teacher points out to students that **for the H₂ molecule to exist, attractive interactions must balance the repulsive ones. When this condition is met, we say that the two atoms are bonded and form a molecule.**

At this point, the teacher can use a version of the Lennard-Jones potential graph in which the dependencies of the attractive and repulsive interactions on the internuclear distance are made explicit (Figure 4.1). Initially the atoms are too far apart to exert a significant mutual influence. At distance d_1 , the positive and negative charges of one atom begin to interact significantly with those of the other atom: they affect each other. Both repulsive and attractive forces act in the system. Their contribution can be represented by the following curves:

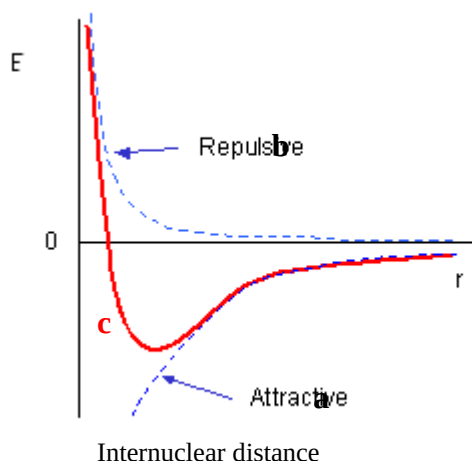


Figure 4.1 - Potential energy vs. internuclear distance in a biatomic system

1. **Curve a** represents the energy variation of the system determined by the attractive interaction between nuclei and electrons, alone. According to Coulomb's law, the resultant of these forces has a **negative** sign and its intensity increases (in absolute value) as the internuclear distance decreases. Therefore, attractive forces cause a decrease in the potential energy of the system.
2. **Curve b** represents the energy variation of the system determined by the repulsive interaction between the two nuclei, and between electrons. According to Coulomb's law, the resultant of these forces has a **positive** sign and its intensity increases as the internuclear distance decreases. Therefore, the repulsive forces cause an increase in the potential energy of the system.
3. The overall dependence of the potential energy of the system on the internuclear distance is defined by **curve c**, which is the resultant of the **algebraic sum** of the energy values of **curve a** and **curve b**. Curve c shows that, as the internuclear distance decreases, the potential energy of the system initially decreases, when the attraction between nuclei and electrons prevails. The lowest energy corresponds to the internuclear distance at which attractive and repulsive forces are balanced: it is an equilibrium point, at which the system is stable. The internuclear distance corresponding to the equilibrium point is called the **bond length**. This condition corresponds to a **minimum of energy**.

At the end of this activity the following conclusions are therefore reached:

- **The interatomic bond inside the H₂ molecule is an electric interaction**
- The bonding condition corresponds to a situation of **equilibrium between forces of opposite sign**.
- The bonding condition corresponds to an **energy minimum of the system**.
- The internuclear distance corresponding to this condition is called **bond length**.

The first point is of considerable importance as one of the general objectives of the entire sequence is precisely to insert all types of bonds within the unifying conceptual framework of their common nature of electrical interactions.

Activity 14

The previous activity highlighted the potential energy change that accompanies bonding in a diatomic system. However, the concept of bonding energy has not yet been formalized.

It is therefore proposed to students to carry out a virtual exercise, by using an app developed by the educational research group of the University of Colorado. This exercise is a consolidation activity for the previously learned concepts: this app allows investigating the dependence of attractive and repulsive interactions in a diatomic system, on the interatomic distance. It also allows checking the factors that influence the depth of the potential well of the Lennard-Jones diagram. This activity allows defining bonding energy in a diatomic system, by rescuing the notions already discussed in WS 7, referred to intermolecular bonding.

Object of the proposed activity	Learning objectives
Virtual experiment on the Lennard-Jones graph	To consolidate the concepts related to the formation of interatomic bonds in molecules. To build the concept of bonding energy for the H ₂ system

Use the following animation: https://phet.colorado.edu/sims/html/atomic-interactions/latest/atomic-interactions_it.html

Select the '*Customize the attraction*' option and use the '*slowed down*' mode. Verify:

1. What happens to the attractive and repulsive forces when you move the atoms apart with respect to the equilibrium distance? (select the attractive and repulsive ones in the '*Forces*' box)

2. What happens to the attractive and repulsive when you move the atoms closer with respect to the equilibrium distance? (select in the '*Forces*' box, the attractive and repulsive ones)

3. Do repulsive forces increase or decrease as distance r decreases?

4. Do attractive forces increase or decrease as distance r decreases (consider their absolute value)?

5. When the balance between attractive and repulsive forces is attained, the energy of the system consisting of the two atoms is:
 - Maximum
 - Minimum
 - I do not know
 - It is not possible to answer

Justify your choice.

-
6. How does the depth of the potential well change by increasing or decreasing the extent of interatomic interaction?

 7. Do you think there is a relationship between the depth of the potential well and the stability of the bond between the two atoms?

 8. Should you wish to take the two atoms apart (from bonding distance to infinite distance) would you need to supply or subtract energy to the system?

At the end of this activity, students are expected to know the dependence of the extent of attractive and repulsive interactions on interatomic distance. After discussion, the classroom is expected to share the following conclusions:

- Whenever the interatomic distance is greater than bond length, the extent of (repulsive and attractive) interatomic interactions is negligible;
- Whenever the interatomic distance is shorter than bond length, repulsive interactions prevails over the attractive ones;
- Upon reaching the balance between attractive and repulsive forces, the biatomic system lies at a minimum of energy (potential well);
- Whenever the extent of interatomic interaction increases, the depth of the potential well increases;
- The deeper the potential well, the more stable the system;
- Atoms may be separated by supplying energy to the system.

Questions 6-8 focus on the potential well, that is, on the energy decrease that characterizes bonding. They aim at making students understand (or consolidate the concept) that an energy decrease involves the stabilization of the system.

Furthermore, the notion discussed in WS 7 are rescued and applied to this new system, in order to get to the definition of bonding energy, as "**the amount of energy that must be supplied to the system in order to separate two bonded atoms and bring them from the bond distance to infinite distance**", that is, to get them out of the potential well. Once the class has shared the idea that, in order to break the bond, energy must be supplied to the system, the quantitative aspect may be tackled one. The teacher asks the class:

- Based on the L-J graph, how much energy must be supplied to the H_2 system so to recover two isolated H atoms?

The aim is to get to the shared conclusion that this amount of energy corresponds to the depth of the potential well. The deeper it is, the more difficult to break the bond; that is, the more stable the system made of two bonded atoms. At this point, the teacher will be able to formalize the definition of bonding energy as "**the amount of energy that must be supplied to the system in order to separate two bonded atoms and bring them from the bond distance to infinite distance; this energy corresponds to the depth of the potential well in the Lennard-Jones diagram**". Consequently, the teacher will point out that the reverse process, that is bonding, always implies a transfer of energy from the system to the environment: that amount of energy is the same that must be supplied to the system to break the bonds. The greater the amount of energy, the more stable the bond.

To reinforce these concepts, the teacher may comment on the following table, that collects bond energy values of several diatomic substances:

SUBSTANCE	BONDING ENERGY (kcal/mol)
H_2	104
F_2	41
Cl_2	58
O_2	117
N_2	225
HF	135
HCl	102
HBr	87
HI	71

If a molecule is polyatomic, the amount of energy needed to break all its bonds and obtain the isolated atoms will be the sum of the energies needed to break each single bond. It corresponds exactly to the amount of energy released to the environment during the formation of that molecule.

Activity 15

It remains to define how to formalize H-H bonding from the microscopic point of view. Students are now aware that interatomic bonding within a molecule is an electrical process that involves the evolution of the system towards a more stable state as compared to the initial condition (isolated atoms). It is therefore necessary to look at the nuclear-electronic level in order to highlight the changes induced by bond formation. Students are asked to imagine how to represent bonding at the nuclear-electronic level, starting from two isolated atoms.

Prior to this activity, students must have dealt with the atomic structure (electron shell model), including the electrons' distribution in the shells (electron configurations) and the differentiation between valence and internal shells.

Object of the proposed activity	Learning objectives
Students are required to represent the formation of the hydrogen molecule at the nuclear-electronic level.	To formalize the bond between two H atoms as the result of the sharing of a pair of electrons.
The electronic configurations of He and H ₂ are compared.	To understand that the stabilization of the system resulting from bonding can be justified in terms of the achievement of electronic configurations similar to that of noble gases.
Students are required to draw up a concept map summarizing what they learnt about the bond found in H ₂ .	To systematize the main concepts related to the formation of the the bond between two H atoms.

Previous activities have shown that two hydrogen atoms can bond together to form a dihydrogen molecule H_2 . When this happens, the resulting system is more stable than the starting one. The interaction between the two atoms is electrical and involves the presence of attractive and repulsive forces, which balanced each other.

1. In the light of these considerations, try to represent the two isolated hydrogen atoms and the H_2 molecule at the nuclear-electronic level.

H Atom

H Atom

 H_2 Molecule

2. How many electrons belong to each H atom once the bond is formed?

3. Represents a Helium atom at the the nuclear-electronic level. How many electrons are found in its electronic configuration?

4. The electron cloud of H_2 and He contains:

- The same number of electrons
- A different number of electrons
- It is not possible to answer
- I can not answer

Justify your answer:

5. Helium is a noble gas and does not combine with other atoms to form molecules: it means that it is a very stable system. Its electronic shell is filled in completely. What happens to the electronic shell of every single H atom when they become part of a H_2 molecule?

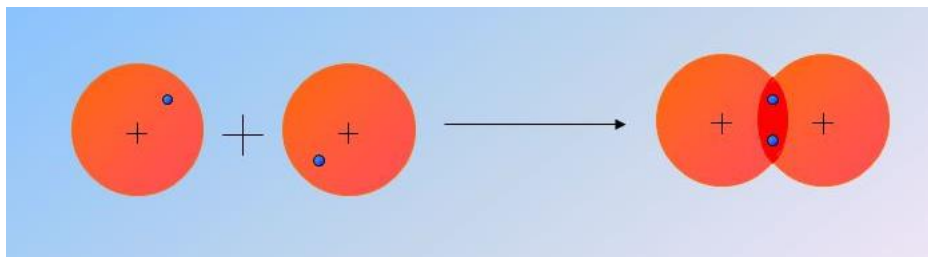
- It is completely filled
- It could host other electrons
- It is not possible to answer
- I can not answer

Justify your answer:

Students are familiar with the atomic shell model and have already used representations of atoms at the nuclear-electronic level. The discussion of WS15 is aimed at suggesting the idea that bonded atoms may share their electrons, i.e. the basis for the Lewis model that will be tackled in subsequent activities. Many students are expected to consider the possibility that the two electrons found in H_2 , as the H atoms approaches may

belong to both atoms. Some students might object that – as electrons are negatively charged - they should repel each other and cannot coexist in the same region of space. The teacher will remind students that the previous activities have highlighted the presence of both repulsive forces between the electrons of each atom, and attractive forces between each nucleus and the electrons in the system. Students have also learnt that, when atoms are bonded, the repulsive and attractive forces counterbalance each other.

The teacher will exploit the discussion in the classroom allow to suggest a bonding model. May the H-H bond found in H_2 be formalized as a shared electron pair between the two H atoms? Such bond can be represented at the nuclear-electronic level in the following way:



The teacher will point out the conventional nature of the above representation: the electron doublet is shared in the sense that it is affected by the attraction of each hydrogen nucleus and moves in a larger space as compared to the isolated H atom. Although this representation is static, the electrons are endlessly moving around the nuclei: the real system is dynamic. Furthermore, the figure does not comply with the real proportions, as the space available to electrons is order of magnitude larger than the nuclear volume.

Once this conclusion is drawn, the teacher will tell students that this bonding model has been developed by scientist and this bonding mode, which is typical of molecular substances, is called **covalent**. In the symbolic language, a shared electron pair, i.e. a covalent bond, is usually represented with a hyphen joining the two bonded atoms:



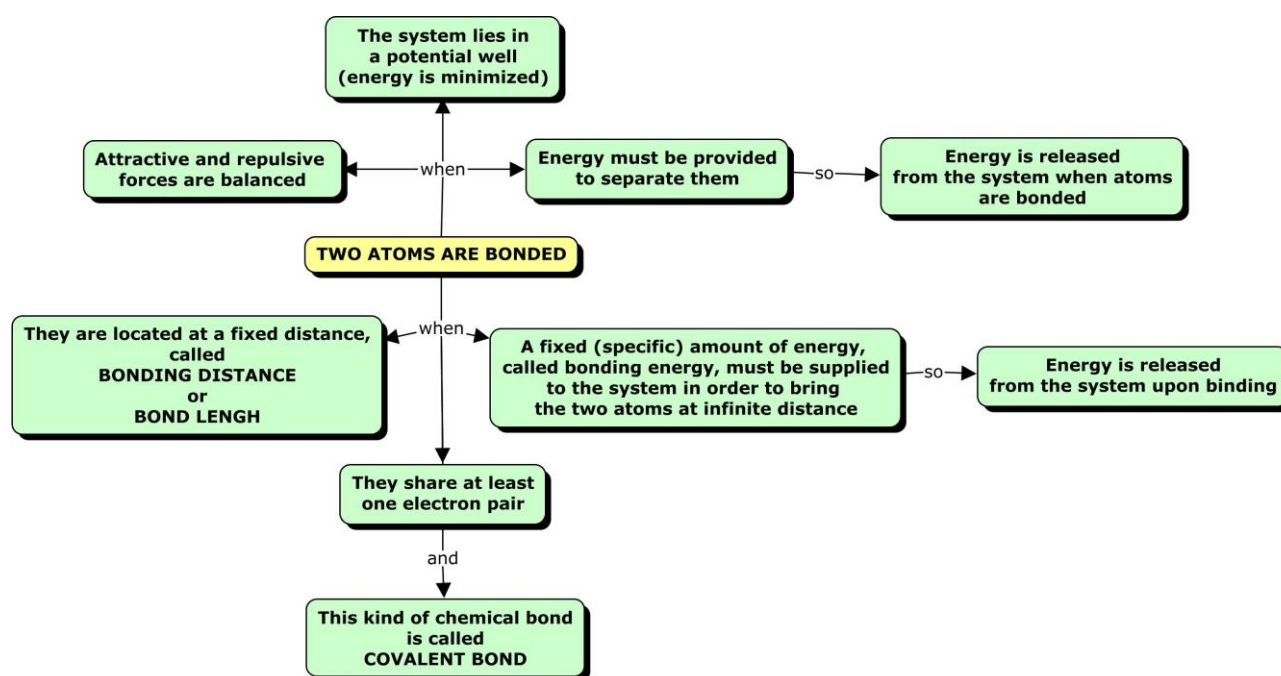
Questions 2-5 aim at clarifying the reasons for the stabilization of the H_2 system as compared to the isolated atoms. The students' answers are discussed in the classroom and the teacher points out that noble gases are not very reactive, that is, they have little or no tendency to combine with other elements of the periodic table. Hence, noble gases are chemically stable. In previous activities, students have learnt that, unlike other elements, noble gases exhibit full valence shells. The teacher suggests students to seek for a correlation between electronic configurations, stability and reactivity. The stabilization of the system that accompanies the formation of the covalent bond can be related to the achievement of full valence shells. In fact, by sharing two electrons, each H atom in the H_2 molecule achieves full valence shell.

In conclusion, the teacher summarizes the properties of the bonding model adopted for the H_2 molecule:

- Substance H_2 is made up of two hydrogen atoms bonded together;
- The bond that holds the two atoms of H together is an electric interaction: it results from the balance of attractive and repulsive interactions;
- When the two H atoms are bonded, their distance is designated as *bond length*;
- When the two H atoms are bonded, the resulting system is more stable (i.e. contains less energy) than the isolated atoms;
- The energy needed to break the bond, that is, to bring the two hydrogen atoms back to an infinite distance, is called *bond energy*;

- The stronger the bond, the greater the bond energy;
- From the nuclear-electronic viewpoint, the H-H bond may be described as a shared electron pair between the two H atoms;
- From the nuclear-electronic viewpoint, the stabilization of the H₂ system corresponds to the achievement of the same electronic configuration as noble gas He (whose outermost shell is completely filled);
- This type of bond is called *covalent bond*;
- This type of bond is represented by a hyphen between the symbols of the two H atoms;
- A hyphen represents a pair of electrons;
- The following representation of the H₂ molecule is called the structural formula: H-H

At the end of this sequence's segment, students receive a homework assignment: they are requested to build up a concept map that summarizes the main concepts involved in covalent bonding. Here is an example of the expected result:

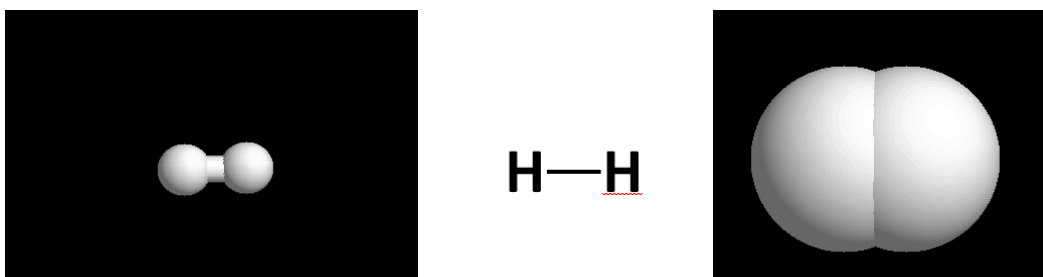


Activity 15 bis (optional)

According to educational research, the *materialization of bonds* is a common misconception, induced by the habit of representing bonds as hyphens, sticks, etc. Visual representations of the atomic-molecular world are essential, as they help highlighting the relationships between microscopic entities. However, misconceptions arise whenever students are unable to discern between a concept and its representation: students do not realise that models and their representations are just tools for reasoning at the microscopic level (atomic-molecular and nuclear-electronic levels). This activity aims at stimulating students to think about the different representations of chemical bonding and to discriminate between the (abstract) concept and its representation.

Object of the proposed activity	Learning objectives
The meaning of various iconic representations of molecules is discussed with students	To reinforce the concept that bonds are immaterial relations. To realize that distinct iconic representations of bonds may have different practical purposes.

To this purpose, we exploit the RASMOL application, which is freely available on the web. The implications of different ways of representing the H₂ molecule are discussed with students. The following figures are shown to students:



The teacher opens the discussion in the class, by stimulating students with some questions, according to how the discussion develops:

- Do these different representations refer to the same object or to different objects?
- What do they represent?
- What is peculiar of each one?
- Do the different representations convey the same information?
- In your opinion, what does the representation of the structural formula highlight? What about the *stick-and-ball* representation? And the spherical model?
- What does the stick represent in the *sticks-and-balls* model?
- Is the bond between two atoms a material object?

The discussion should help students realize that a same microscopic object (i.e. the dihydrogen molecule) may be represented in several ways: this is possible because the object and its representations do not coincide. These are just visualizations of molecular models. The representations change according to the aim which is pursued: if I need to think about the molecular volume, the spherical model fits well; if I just need to highlight that the H atoms are bonded, the simple structural formula will be OK, etc...

The teacher will then underline the fact that the dash represented in the structural formulas or the stick found in the *sticks-and-balls* models are material representations of an immaterial relationship, the chemical bond. Bond is a synonym of preferential relationship between atoms. A relationship is not a material link, like a rope that holds two macroscopic objects together. We need signs (the hyphen) or material symbols (the stick) to represent their existence. By analogy, it is possible to compare interatomic bonds with the relationship between the Sun and the planets of the solar system: the forces acting between the planets and the Sun are immaterial, yet we recognize that they are bound together. Similarly, atoms are bonded by electrical forces. These are not material constraints, but we need to represent them with conventional signs, to highlight their presence.

Activity 16

This activity aims at pointing out that intramolecular bonding perturbs atoms' electronic structure, i.e. it modifies their outermost electron shell. It is therefore necessary to consolidate the difference between electrons of the outermost shell and electrons of the inner shells.

Object of the proposed activity	Learning objectives
Students are asked to represent the electron shells of fluorine and chlorine atoms and to establish which electrons participate in the covalent bond found in F_2 and Cl_2 molecules.	To understand that intermolecular bonding (hence, chemical reactivity) perturbs only the outermost shell of atoms. To consolidate the concept that bonding goes along with the stabilization of the system, which can be explained with the achievement of full outermost shells of the bonded atoms.

WS 16A

Experimental data tell us that:

- The difluorine molecule is made up of two fluorine atoms bonded together: its chemical formula is F_2 .
- The dichlorine molecule is made up of two chlorine atoms bonded together: its chemical formula is Cl_2 .

1. Represent a fluorine atom and a chlorine atom at the nuclear-electronic level by using the atomic model that you have learnt (with the electrons distributed in electron shells):

FLUORINE

CHLORINE

2. In the light of what you learnt about the atomic structure, how many electrons does fluorine have in its outermost shell? How many electrons are part of the inner shells?

3. In the light of what you learnt about the atomic structure, how many electrons does chlorine have in its outermost shell? How many electrons are part of the inner shells?

We defined the covalent bond as the sharing of an electron pair by two atoms that are placed at equilibrium distance.

4. Represent a difluorine molecule at the nuclear-electronic level by using the atomic model that you have learnt (with the electrons distributed in electron shells):

5. Represent a dichlorine molecule at the nucleus-electron level at the nuclear-electronic level by using the atomic model that you have learnt (with the electrons distributed in electron shells):

6. In the previous representations, does the number of electrons in the chlorine inner shells change after the bond is formed? And does the number of electrons in the fluorine inner shells change?
- Yes, it changes
 - No, it does not change
 - I do not know
 - It is not possible to answer

Justify your answer:

7. In the previous representations, does the number of electrons in the outermost shell of chlorine change after the bond is formed? And does the number of electrons in the outermost shell of fluorine change?
- Yes, it changes
 - No, it does not change
 - I do not know
 - It is not possible to answer

Justify your answer:

8. In the previous representations, how many electrons do you assign to the outermost shell of each chlorine and fluorine atom before and after the bond is formed?

CHLORINE:	BEFORE.....	AFTER.....
FLUORINE:	BEFORE.....	AFTER.....

9. How many electrons are shared by the two fluorine atoms in the difluorine molecule?
- Two electrons
 - More than two electrons
 - All valence electrons
 - I do not know
 - It is not possible to answer

Justify your answer:

10. How many electrons are shared by the two chlorine atoms in the dichlorine molecule?
- Two electrons
 - More than two electrons
 - All valence electrons
 - I do not know
 - It is not possible to answer

Justify your answer:

11. Compare the number of electrons in the outermost shell of fluorine after the formation of the F-F bond with the valence electrons of Ne. What do you notice?

12. Compare the number of electrons in the outermost shell of chlorine after the formation of the Cl-Cl bond with the valence electrons of Ar. What do you notice?

13. In FOL 15 we noticed that each H atom inside the H_2 molecule had the same electronic configuration of the noble gas He. The stability of the H_2 system was associated to this fact. In your opinion, can something similar happen in the Cl_2 and F_2 molecule?

- Yes, it can
- No, it cannot
- I do not know
- It is not possible to answer

Justify your answer:

Questions 2-5 focus on the difference between inner shells and outershell electrons in atoms. Students might already know this distinction, from their previous study of atomic structure (electron shell model).

Questions 6-8 aim at making student realise that – according to the same rationale applied to the formation of the H_2 molecule - F_2 and Cl_2 formation implies perturbation of just the outermost shell of fluorine and chlorine atoms: their inner shells keep unperturbed.

Questions 9-10 highlight that F-F and Cl-Cl bonding implies sharing of an electron doublet from the outermost shell.

Questions 11-13 seek for a justification of this bonding model: by analogy with H_2 , it is shown that F and Cl atoms may achieve a noble gas configuration by sharing a single electron pair. Since the previous activities:

- have established a **relationship** between electronic configurations and the energetic stability of the system.
- have established that bonding implies the **stabilization** of the system.

the formation of F_2 and Cl_2 may be justified in terms of stabilization deriving from the achievement of full outermost shells, as it occurs in noble gases.

Students may wonder about the reasons for the different behavior of inner shells vs. outer shell electrons. The teacher recalls what students learnt from previous activities on electrical interactions and atomic structure: the electrons of the outermost shells are less attracted by the atomic nucleus as compared to inner shells electrons; in addition they are closer to the partner atom and feel its attraction. Conversely, inner shells electrons are firmly bound to the nucleus of the atom to which they belong.

At the end of this activity, the teacher summarizes the outcome of the classroom discussion, by generalizing the statements previously referred to the H_2 molecule:

- Diatomic substances such as H₂, F₂ and Cl₂ are formed by two atoms interacting through *covalent bonds*.
- This bond is an electric interaction and it results from the balance of attractive and repulsive interactions;
- The distance between the two bonded atoms is called the *bond length*
- When the two atoms are bonded, the resulting system is more stable (i.e. contains less energy) than the isolated atoms;
- The energy needed to break the bond, that is to bring the two atoms back to an infinite distance, is called the *bond energy*.
- The stronger the bond, the greater the bond energy.
- From the nuclear-electronic viewpoint, covalent bonding consists in sharing an electron pair between the two bonded atoms.
- From the nuclear-electronic viewpoint, covalent bonding involves only electrons from the outermost shell of atoms.
- The electrons of the inner shells do not play any role in covalent bonding.
- From the nuclear-electronic viewpoint, the stabilization of the molecular system corresponds to the achievement of the same electronic configuration as noble gases, that is, to the completion of the outermost electron shell.
- The covalent bond is represented with a hyphen between the symbols of the two bonded atoms.
- A hyphen represents a pair of electrons;
- The representation of how atoms are linked together to form a molecule is called the *structural formula*.

Activity 17

Object of the proposed activity	Learning objectives
The rules of the Lewis model are set out, based on the conclusions of the previous activity.	To understand the meaning of the Lewis model. To learn how to build structures of simple molecules through the rules of this model.

Once the notion of covalent bond (and its related concepts) built up through the discussion of simple diatomic molecules, it becomes necessary to extend its field of application and move on to molecules of greater complexity. The discussion of the results of the previous activity allowed the teacher to point out that only outer shell electrons are involved in covalent bonding, whereas inner shell electrons are strongly attracted by the positively charged nucleus: they constitute the atom's *core or kernel*. This notion can be discussed with reference to Lewis' words (Lewis 1916):

1. *In every atom is an essential kernel which remains unaltered in all ordinary chemical changes and which possesses an excess of positive charges corresponding in number to the ordinal number of the group in the periodic table to which the element belongs.*
2. *The atom is composed of the kernel and an outer atom or shell, which, in the case of the neutral atom, contains negative electrons equal in number to the excess of positive charges of the kernel.*

It is then possible to introduce the Lewis model for the determination of the electronic structures of molecules. Once the latter have been obtained, the application of the VSEPR theory will allow to obtain information on the spatial arrangement of atoms, that is, on molecular geometry. This activity aims at stating the Lewis'

model rules and using them for building the structural formulas of simple molecules (halogens, water, ammonia, dioxygen and dinitrogen). Clearly, the Lewis model is not 'built' by students: it is proposed by the teacher. In carrying out this activity, the teacher must highlight the rationale of the model, by recalling the conclusions of previous activities carried out in the classroom (e.g. WS 16). Students already know what is a model and should be aware of its interpretive and predictive function: the Lewis model can be proposed by highlighting precisely these features.

The relationship between the stability of an atomic-molecular system (energetic factors) and the electronic configurations of its constituent atoms has already been discussed in previous activities. The system stability has also been related to its reactivity. Noble gases, which have complete valence shells, are not reactive (or very little reactive): they are stable systems. Atoms with incomplete valence shells bind other atoms to achieve a similar condition as noble gases, i.e. to complete its valence shell.

These statements form the interpretive basis of the Lewis model, i.e. the so-called **octet rule**.

To illustrate this rule, the teacher represents the atoms of the main groups of the Periodic Table as follows:

The chemical symbol indicates the atom's kernel; the core is surrounded by as many electrons as those found in the outermost atomic shell.

Lewis Periodic Table Showing Outer Shell (Valence) Electrons

1	2	3	4	5	6	7	8
H•							•He•
Li•	•Be•	•B•	•C•	•N•	•O•	•F•	•Ne•
Na•	•Mg•	•Al•	•Si•	•P•	•S•	•Cl•	•Ar•
K•	•Ca•	•Ga•	•Ge•	•As•	•Se•	•Br•	•Kr•
Rb•	•Sr•	•In•	•Sn•	•Sb•	•Te•	•I•	•Xe•
Cs•	•Ba•						

<https://archivioscienze.scuola.zanichelli.it/esperto-chimica/2013/01/25/le-formule-di-lewis/>

Then, the teacher writes the brute formulas of some substances (in the form $A_xB_yC_z$) and engage students in the construction of molecular structures according to the Lewis model.

The Lewis model is built on the following assumptions:

1. When two or more atoms bind to each other, their electronic configuration changes and becomes similar to that of the closest noble gas, as this corresponds to a more stable situation as compared to the starting one.
2. When two or more atoms bind to each other, the electrons of the outer shells are shared so as to allow each atom to achieve a full shell configuration.
3. Each bond between two atoms corresponds to a shared electron pair and is represented by a hyphen (or two points) between the two atoms.
4. Each unshared electron pair belonging to a given atom is represented by a hyphen (or two points) next to the corresponding atomic symbol.

From the operational viewpoint, the procedure requires:

1. To consider the brute formula ($A_xB_yC_z$) of a substance.
2. To calculate the total number of valence electrons available for bond formation in the molecule. Valence electrons of each single atom in the molecule are summed up.
3. This number is divided by two: this provides the number of electron pairs in the molecule.
4. Electron pairs are distributed on the atoms in the molecule, so that all the atoms are bound together (i.e. each atom must share at least one pair of electrons with another atom).
5. In doing so, one has to make sure that all the atoms in the molecule achieve a full outermost electron shell. Some electron pairs are shared between two atoms and represent covalent bonds (bonding pairs). Others belong to a single atom and are not involved in bonds (non-bonding pairs). This step ensures that all atoms reach a stable condition.
6. At the end, the overall sum of the electron pairs in the molecule must equal the number identified in step 3.

The proposed model avoids to define and apply the notion of formal charge, as we believe it unnecessary at this school level. It is a formal concept and students would hardly understand its meaning. Furthermore, the notion of formal charge is useful especially for resonance formulas, that won't be tackled at this school stage. The class will spend some time in learning how to apply the Lewis model and the octet rule. The teacher leads the class in building up the Lewis' structure of simple substances such as F_2 , H_2O , CH_4 , etc. Molecules with double and triple bonds will also be discussed. This helps clarifying **the meaning of bonding and non-bonding electron pairs and to point out the possibility of having multiple electron pairs shared between atoms**.

Once the class is sufficiently trained, students are assigned homeworks such as the following one.

WS 17

By applying the previously stated rules, determine the structural formulas of Cl_2 , HCl , NH_3 , H_2S , C_2H_6 , O_2 , CO_2 , N_2 , HCN according to the Lewis model. These molecules are all linear (they are not cyclic) and all atoms comply with the octet rule.

At the end of this activity, the teacher checks the outcomes of students' homework and discusses them with students.

We'd like to stress the relevance of the octet rule, introduced with this activity. In fact, all subsequent chemical bonding models will refer to this rule, whose meaning is related with the previously discussed energetic factors and the stability deriving from the achievement of full electron outer shells. Hence, we avoid using the octet rule as teleological explanation; we rather connect it to the energetic stability of the system, which is the rationale behind all the transformations examined in this sequence.

Of course, just like any other model, Lewis' model has descriptive/explanatory limitations. These limits must be taken into account and highlighted the discussion of specific cases, known as "*exceptions to the octet rule*" (e.g. AlH_3 , SO_3 , etc.).

Activity 18

Once the concept of *covalent bond* has been built, the concept of polarity remains to be addressed.

In order to build it, it is necessary to resort to ancillary concepts, such as electronegativity. Students might already know this concept from previous discussions of the periodic properties of elements. If they don't, this notion needs to be introduced in this context through specific activities.

The identification of the polarity of substances is highly relevant in chemistry, as polarity influences (either directly or indirectly) properties such as: their solvent power, their physical state at a given temperature and pressure, etc.

Since this teaching sequence insists on building up/presenting microscopic models as explanatory tools, i.e. reasoning tools that allow interpreting the macroscopic behavior of material systems, we believe important to introduce the notion of *polarity of substances* from empirical observations on their behavior.

Object of the proposed activity	Learning objectives
The effect of two rods - electrified in opposite ways - on the flow of a polar and a non-polar substance is empirically verified and discussed.	To capture the different behavior of polar and non-polar substances in the presence of an electric field. To stimulate the search for a microscopic interpretation of this phenomenon.

Students are engaged in an experiment during which two substances exhibit distinct behaviors face to the same solicitation. Student are faced to a problem-situation that needs resorting to the microscopic, atomic-molecular and nuclear-electronic levels. Due to substance toxicity, the experiment is proposed in the form of a video recording that shows the different behavior of two liquids, a polar one (ethyl alcohol) and a non-polar one (tetrachlorethylene), placed under the action of an electric field. Two opposite electric field are generated by rubbing a glass rod and an ebonite rod with a wool cloth. The two substances are placed in two burettes and the liquid is slowly dripped, next the electrified rods. Both rods attract the polar liquid, whereas the non-polar liquid is insensitive to the presence of the two rods.

These distinct behaviors qualifies the two substances as systems with different electrical properties. The two substances are also mixed to water. Seemingly, their distinct behavior towards water qualifies them as hydrophilic and non-hydrophilic (or lipophilic). How to interpret their dual behavior?

Consider two liquid substance A and B. Perform the following actions:

1. Pour each liquid into a burette previously treated with a few milliliters of the same liquid
2. Rub a glass rod and an ebonite rod with a wool cloth. They get electrified positively and negatively, respectively
3. Drip one liquid at a time, collecting it in a beaker. While dripping, alternately bring the glass rod and the ebonite rod close to the stream that comes out of the burette.
4. Record what you observe and write it down in the table below.

	Liquid A	Liquid B
Ebonite		
Glass		

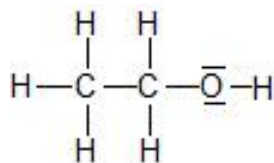
5. Do liquid A and liquid B display the same behavior?
 - Yes, they do
 - No, they don't.
 - I do not know
 - It is not possible to answer
6. Try pouring a little bit of liquid A into water, into a sample tube. Does it mix easily?
 - Yes, it does
 - No, it does not
 - I do not know
 - It is not possible to answer
7. Try pouring a little bit of liquid B into water, into a sample tube. Does it mix easily?
 - Yes, it does
 - No, it does not
 - I do not know
 - It is not possible to answer
8. In the laboratory reagentary you can find acetone and ethyl ether. Check if they behave like substance A or B with water

	It mixes with water	It does not mix with water
Acetone		
Ethyl ether		

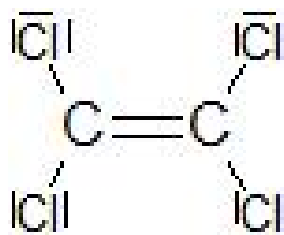
After looking at these videos and let students the time to fill WS18 in, the teacher summarises the experimental findings: substance A is affected by the electrified rods, whereas substance B is not. Hence, an electrical phenomenon is involved (*please note that students are familiar with electrostatics*). In addition, substance A and acetone can be mixed to water: they are *hydrophilic* substances). Conversely, substance B and ethyl cannot, they are *non-hydrophilic* (or *lipophilic*) substances.

How can these behaviors be interpreted? The discussion should lead students to conclude that, in the light of previous experiences, the explanation of these phenomena must be sought at the microscopic level. It is necessary to know how the molecules of these substances are made in order to decipher their behavior.

Sensitivity to charges suggests to look at how electrons are distributed in these molecules. So, the Lewis structures of substance A and B may help solving the problems. These structures are then showed to students.



Ethyl alcohol (A)



Tetrachlorethylene (B)

The teacher will point out to the students that these substances are made up of atoms of different elements (contrary to F_2 , H_2 , etc. examined previously). The teacher asks: *May the presence of different types of atoms affect the way these atoms are bonded?*

Activity 19

This activity introduces the hypothesis that the shared electron pair that we call *covalent bond* may not be shared equally, i.e. electron sharing is asymmetrical. To qualify this asymmetry, the notions of *electronegativity* and *bond dipole* need to be introduced. Then, the behavior of the substances of WS18 will be re-examined. Substances A and B will then be classified as *polar and non-polar*, depending on the presence or absence of *permanent molecular dipoles*.

Object of the proposed activity	Learning objectives
The diatomic substances H_2 and HCl are compared: a qualitative assessment of the extent of attractive and repulsive forces at play within them is made	To understand that the <i>cores</i> of different elements attract bonding electrons to a different extent, due to their distinct charge.

The starting question for this activity is the same with which the previous activity ended: *May the presence of different types of atoms affect the way these atoms are bonded?* Two covalent diatomic substances, H_2 and HCl , are compared and the consequences of replacing an H atom with a Cl atom are discussed.

We learnt that a covalent bond is found in both the dihydrogen molecule and the hydrogen chloride molecule. This bond consists of a shared electron pair between the two bonded atoms. In the molecules of each of these two substances, the two bonding electrons are attracted by both the atomic kernels of each atom 1 and 2, as these kernels are positively charged.

1. In your opinion, in the dihydrogen molecule:

- Kernel 1 attracts bonding electrons as much as kernel 2
- Kernel 1 attracts bonding electrons at a different extent than kernel 2
- I do not know
- It is not possible to answer.

Justify your answer.

2. In your opinion, one can say that in the dihydrogen molecule:

- The two bonding electrons, in their endless movement, spend the same amount of time near kernel 1 and kernel 2
- The two bonding electrons in their endless movement, spend a different amount of time near kernel 1 and kernel 2
- I do not know
- It is not possible to answer.

Justify your answer.

3. In your opinion, in the hydrogen chloride molecule:

- The H kernel attracts bonding electrons as much as the Cl kernel
- The H kernel attracts bonding electrons to a different extent as compared to the Cl kernel
- I do not know
- It is not possible to answer.

Justify your answer.

4. In your opinion, one can say that in the hydrogen chloride molecule:

- The two bonding electrons, in their endless movement, spend the same amount of time near the H kernel and the Cl kernel
- The two bonding electrons in their endless movement, spend a different amount of time near the H kernel and the Cl kernel
- I do not know
- It is not possible to answer.

Justify your answer.

5. What is the charge of the H kernel?

6. What is the charge of the Cl kernel?

The issues addressed in this sheet should not be too difficult to students, as they are accustomed to think in terms of electric attractions and repulsions. The classroom discussion, led by the teacher, should lead students to share the following ideas:

- In the H₂ molecule, the two atomic cores are identical and therefore attracts the bonding electrons to the same extent. One can say that bonding electrons, in their endless motion, spend the same amount of time next to core 1 and core 2.
- In the HCl molecule, the two cores are different and exhibit different charges. The charge of Cl is greater than that of H. Therefore, the chlorine core exerts a stronger attraction towards the bonding electrons. One can say that bonding electrons, in their endless motion, spend different amounts of time next to the two atomic cores of H and Cl.

The teacher will remark the purely qualitative character of these statements. Is it possible to establish a quantitative criterion that allows 'quantifying' the different distribution of electrons among the atomic cores in a molecule?

Activity 20

The previous activity introduces the idea that electron sharing in a covalent compound may not be symmetrical, due to the different extents of the attraction exerted by distinct atomic cores in the molecule. It is now matter of understanding which criteria can help predicting the presence of such an asymmetry and how it can be quantified. To this purpose, *electronegativity* is introduced. It can be **qualitatively** defined as the tendency to attract bonding electrons, typical of each atom within a molecule. The teacher then proposes a **quantitative definition** of electronegativity. We believe that the most affective choice in this school context Mulliken's. In fact, Mulliken calculates electronegativity as the average of two experimentally determined quantities that are familiar to students as periodic properties: the ionization energy and the electron affinity. Hence, Mulliken's electronegativity is easier to understand than Pauling's (albeit it's being the most widely used).

Object of the proposed activity	Learning objectives
Qualitative and quantitative definitions of electronegativity are proposed using the Mulliken scale	To learn the concept of electronegativity and to understand its meaning.
Students are asked to calculate the electronegativity difference between the atoms of different molecules and to identify the bonds characterized by an asymmetric sharing of bonding electrons.	To use electronegativity values of the elements to predict whether a covalent bond is characterized by a symmetrical or asymmetric sharing of bonding electrons between two bonded atoms. To define criteria for discriminating between polar and non-polar bond.

The teacher, based on WS 19, states that "the tendency of an atom in a molecule to attract bonding electrons" has been quantified by researchers through a parameter called *electronegativity*. This tendency depends on various factors, including the nuclear charge, the number of electrons in the atomic core, and the energy required to move an electron apart from an isolated atom or to insert an electron into an isolated atom, i.e. *first ionization energy* and *electronic affinity*, two parameters whose meaning is already known to students.

The teacher introduces the quantitative definition of electronegativity proposed by Mulliken. Mulliken's electronegativity is defined as the average of the ionization energy and the electronic affinity of an element:

$$EN = (EI + AE)/2$$

By using the periodic table, the teacher comment on the periodic trend of this parameter to the students. Calculations show that the most electronegative elements belong to groups VI and VII (especially the elements at the top right of the periodic table) as they are characterized by a high ionization energy and a high electronic affinity. Conversely, the least electronegative elements are the metals of groups I and II groups (especially those at the bottom left of the periodic table). The teacher points out that other quantitative definitions have also been proposed by other researchers: therefore, various electronegativity scales are available. Although they show different numerical values, all electronegativity scales show the same periodic trend. Once Mulliken's electronegativity defined, the teacher proposes the following worksheet to the students.

Electronegativity of an element can be defined as the tendency of an atom (bonded to another atom) to attract bonding electrons.

The greater the difference in electronegativity between two atoms bound together, the more asymmetrical their sharing of bonding electrons. Take a look at the following electronegativity values calculated by Mulliken:

1	H 2,25																	He 3,49
2	Li 0,97	Be 1,54										B 2,04	C 2,48	N 2,90	O 3,41	F 3,91	Ne 4,49	
3	Na 0,91	Mg 1,37										Al 1,61	Si 1,90	P 2,19	S 2,69	Cl 3,10	Ar 3,49	
4	K 0,73	Ca 1,08	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu 1,49	Zn 1,68	Ga 2,01	Ge 2,33	As 2,26	Se 2,60	Br 2,95	Kr 3,00
5	Rb 0,69	Sr 1,00	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag 1,47	Cd 1,53	In 1,76	Sn 2,21	Sb 2,12	Te 2,41	I 2,74	Xe 2,73
6	Cs 0,62	Ba 0,88	*	Hf	Ta	W	Re	Os	Ir	Pt	Au 1,87	Hg 1,81	Tl 1,96	Pb 2,41	Bi 2,15	Po 2,48	At 2,85	Rn 2,59
7	Fr 0,68	Ra 0,92	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og

1. Assigning each element its own electronegativity value and calculate the electronegativity difference between bonded atoms in the following molecules, corresponding to the substances examined in WS 17:

Molecule	Bonds	Difference in electronegativity
Cl ₂	Cl-Cl	
HCl	H-Cl	
NH ₃	N-H	
H ₂ S	H-S	
C ₂ H ₆	C-C	
C ₂ H ₆	C-H	
O ₂	O-O	
CO ₂	C-O	
N ₂	N-N	
HCN	C-N	
HCN	C-H	

2. Which bonds display the greatest difference in electronegativity?

3. Which bonds display a zero electronegativity difference?

4. Based on what we learnt from WS 18, which bonds in the table are characterized by an asymmetrical sharing of bonding electrons?

5. Based on what we learnt from WS 18, which bonds in the table are characterized by a symmetrical sharing of bonding electrons?

Students' answers are discussed in the classroom.

The teacher points out that, whenever bonds involve atoms with $\Delta_{\text{Electronegativity}} = 0$, the bonding electrons are equally shared between the two atoms. Conversely, whenever bonds involve atoms with $\Delta_{\text{Electronegativity}} \neq 0$, the bonding electrons are asymmetrically shared between the two atoms; in other words, bonding electrons spend more time around the more electronegative nucleus. The dipole notion, built in previous activities, has to be recalled: the asymmetric sharing of bonding electrons between two atoms corresponds to systems where the barycentres of the positive and negative charges do not coincide. Therefore, the system is a dipole. As the asymmetry is permanent, we call it a **permanent dipole** and we say that **the bond is polarised**. The extent of polarisation depends on $\Delta_{\text{Electronegativity}}$.

Conversely, the symmetric sharing of bonding electrons between two atoms correspond to systems where the barycentres of the positive and negative charges coincide. In this case, there is no dipole and the bond is not polarised.

In summary, in the first case a **polar covalent** bond is established between two atoms; in the latter case a **non-polar covalent bond** is formed.

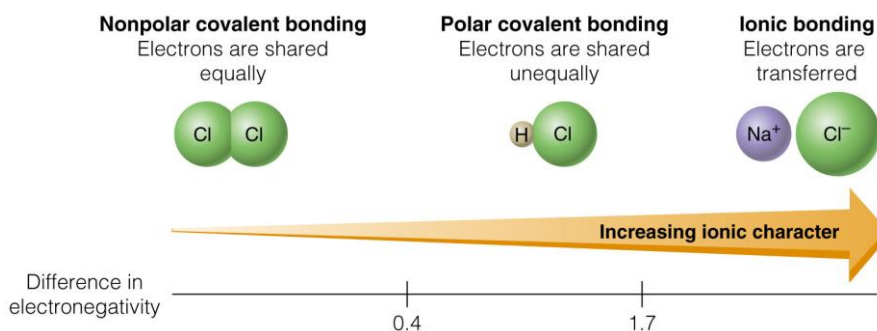
It should be borne in mind that dipole concept has already been built in the initial activities of this sequence and therefore is already familiar to students. The teacher discusses with students the difference between instantaneous dipoles found in noble gases or in H_2 , F_2 , etc. and permanent dipoles. In both cases, an asymmetric distributions of the electron charge occur over time. However, in the present case this distribution is not temporary, but permanent, by virtue of the electronegativity difference of the elements involved in the bond. Finally, the teacher will recall that asymmetrical charge distribution within a neutral system is highlighted by signs δ^+ and δ^- .

Students can now establish which chemical bonds are more polarised, among those listed in WS 20.

In fact, bond polarity is proportional to $\Delta_{\text{Electronegativity}}$: the greater the difference in electronegativity between the bonded atoms, the greater the asymmetry in the distribution of bonding electrons, the greater the polarity. In conclusion, the teacher summarises the content of this lecture as follows:

- A shared electron pair between two atoms is called a **covalent bond**, according to Lewis' model.
- Bonding electrons are attracted by the cores of both bonded atoms.
- Whenever bonding electrons are equally attracted by the two cores, they spend the same amount of time next to each core. Hence the barycentres of positive and negative charges in the system coincide. The bond is said to be **non-polar covalent**.
- Whenever bonding electrons are attracted by the two cores to a different extent, they spend more time next to one core as compared to the other. Hence, the centers of positive and negative charges in the system do not coincide. We call it a **permanent dipole**. The bond is said to be **polar covalent**.
- The parameter that allows evaluating the tendency of an element to attract bonding electrons is called **electronegativity**.

Bond polarity is here directly correlated to $\Delta_{\text{Electronegativity}}$ between the bonded atoms. This is a very common statement, found in all general chemistry. Usually, bonds are classified in textbook based on specific ranges of $\Delta_{\text{Electronegativity}}$:



https://wps.prenhall.com/wps/media/objects/439/449969/Media_Portfolio/ch08.html

This simplification is very useful as a guideline, but it has limitations. For example, sodium bromide $NaBr$ and hydrofluoric acid HF are respectively ionic and covalent substances, despite exhibiting $\Delta_{\text{Electronegativity}} = 1.9$ in both cases. In this case, the criterion based on $\Delta_{\text{Electronegativity}}$ fails. Nahum et al. (2008) remark the partiality of this criterion and recall that bond polarity depend on various factors (e.g. the atomic size).

Activity 21

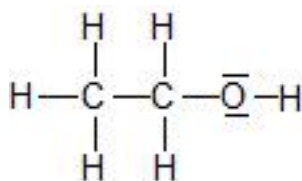
Once the concept of *bond polarity* tackled, it is necessary to move on to the molecular level and to build the concept of *molecular dipole*. This implies establishing a logical connection between these two notions. Students know that dipole is always the result of an asymmetric charge distribution: this is true at both the bond and the molecular level. In order to predict the polarity of molecule, the notion of *molecular geometry*

has to be introduced. Finally, students will learn how to apply the concept of molecular dipole (which refers to the atomic-molecular and nuclear-electronic levels) for interpreting the macroscopic behavior of substances placed in an electric field (i.e. the experiment carried out in WS 18).

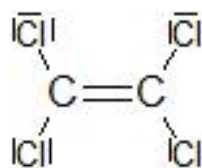
To introduce the problem, it is possible to resort to the structural formulas of substances A and B from WS18.

Object of the proposed activity	Learning objectives
The structural formulas of substances A and B from WS18 are examined: students are asked to identify polar and non-polar bonds within these molecules. Students seek a criterion that allows interpreting their different behavior in the presence of an electric field	To understand that bond polarity is a necessary but insufficient criterion for predicting the behavior of substances in electric fields To introduce the concept of molecular geometry.

Examine the molecules corresponding to substances A and B of WS 18



Ethyl alcohol (A)



Tetrachlorethylene (B)

1. In the light of what you learnt about polar and non-polar covalent bonds, summarize in the following table which polar and non-polar bonds are present in these two species, using the difference in electronegativity as a predictive criterion.

Ethyl alcohol	Tetrachlorethylene

2. Was substance A sensitive to the electric field?
- Yes it was
 - No it was not
 - I do not know
 - I do not remember
3. Substance A has:
- Polar bonds only
 - Non-polar bonds only
 - Both types of bond
 - I do not know
4. Was substance B sensitive to the electric field?
- Yes it was
 - No it was not
 - I do not know
 - I do not remember
5. Substance B has:
- Polar bonds only
 - Non-polar bonds only
 - Both types of bond
 - I do not know
6. Can you establish a criterion that allows interpreting the different behavior of substances A and B under the action of an electric field?

Students are expected to use their knowledge on polar and non-polar bonds to interpret the behavior of substances A and B. Possibly, some students propose the absence or presence of polar bonds in molecules as a criterion for predicting how a substance behaves under the effect of the electric field (question 6). The teacher points out that both molecules A and B contain polar bonds, but substance A is sensitive to the electric field, whereas substance B is not. The proposed criterion is insufficient.

Other students might remark the presence of multiple bonds in substance B and suggest it as a criterion. The teacher invites students to take molecular structure into account and engages students in activity 22: the analysis of various molecular structures might help identifying the interpretative criterion they are looking for.

Activity 22

Goal of this activity is to examine the Lewis structures of various substances and to identify a classification criterion, that is, to build general categories of Lewis structures.

Given the general formula AX_mE_n (where A represents the central atom of a molecule, X represents the atom or atoms bonded to atom A and E represents non-bonding electron pair/s, whose number is given by m and n), molecules can be assigned to the following sets: AX_2 , AX_3 , AX_4 , AX_2E , AX_3E and AX_2E_2 .

In order to achieve this result, students are engaged in the construction of the Lewis structures of the following molecules: $BeCl_2$, CO_2 , BF_3 , BCl_3 , $AlCl_3$, SO_3 , CH_4 , CCl_4 , SO_2 , O_3 , NH_3 , PCl_3 , H_2O , H_2S . The results are shared with the classroom and students are asked to group substances according to a criterion of structural similarity: for example, species as $BeCl_2$ and CO_2 are expected to be assigned to the same set. At the end of this activity, the teacher illustrates the AX_mE_n symbology and shows how to apply it to the sets previously established by students. In other words, students are engaged in a generalisation activity, aimed at defining categories: AX_2 , AX_3 , AX_4 , AX_2E , AX_3E and AX_2E_2 .

The problem requires to spot out at least 6 different categories. However, WS 22 contains a 4-row table; this is made purposely, to check whether students realise that further row have to be added.

Object of the proposed activity	Learning objectives
The Lewis structures of various substances are determined. Categories corresponding to specific electronic geometries are constructed	To understand that the variety of Lewis structures can be traced back to some general categories, namely AX_mE_n (AX_2 , AX_3 , AX_4 , AX_2E , AX_3E and AX_2E_2)

1. Build up the Lewis structures of the following molecules: BeCl_2 , CO_2 , BF_3 , BCl_3 , AlCl_3 , SO_3 , CH_4 , CCl_4 , SO_2 , O_3 , NH_3 , PCl_3 , H_2O , H_2S
2. Can you imagine a criterion according to which these structures can be grouped in different sets? Can you arrange the structures in the table below, according to the criterion you have chosen? Each set must contain molecules that, in your opinion, meet the same criterion (you shall decide how many sets are needed):

Set 1			
Set 2			

3. Which classification criterion have you identified?

At first, the teacher checks if the Lewis structures proposed by students are correct.

Then, the classification criteria proposed by the students are discussed and compared. Many students are expected to propose a criterion based on the number of atoms bonded to the central atom. The teacher points out that non-bonding electron pairs may also be taken into account and invites students to modify their classifications accordingly. By adopting this further criterion, two more rows must be added to the table: the teacher remarks the relationship between molecular structure and distribution of both bonding and non-bonding electron pairs. At the end of this activity, the teacher proposes the general formula AX_mE_n , where A represents the central atom of the structure, X represents a pair of bonding electrons, E represents a pair of non-bonding electrons. To indicate the number of bonding and non-bonding electron pairs belonging to atom A, subscripts can be used: for example, the formula AX_2E_2 indicates a generic Lewis structure with 2 bonding pairs (i.e. two atoms are bonded to atom A) and 2 non-bonding pairs. The teacher finally asks students to classify molecules according to this symbolism. The following groups will result: AX_2 , AX_3 , AX_4 , AX_2E , AX_3E and AX_2E_2 .

Activity 23

The limit of Lewis formulas is that they are two-dimensional representations of three-dimensional entities: students need to understand that the spatial arrangement of atoms symbolized by Lewis structures is, in fact, three-dimensional. Didactic games for the construction of structural models can be employed to this purpose (Warfa et al. 2014).

The goal of this WS is to transpose structural classes AX_mE_n in the 3D space through the GEOMAG game. In the absence of GEOMAG, it is possible to rely on structures made of polystyrene or plasticine balls and toothpicks. By using ball-and-sticks models, students are introduced to the basic rules of the VSEPR theory, i.e. the idea that electron pairs are arranged as far away as possible from each other to minimize repulsions.

During this activity, the teacher reminds students that sticks are mere representations of shared electron pairs (see WS 15 bis). Based on the students' knowledge on electrostatics, the teacher remarks that, due to their negative charge, electron pairs repel each other. To minimize repulsion, the pairs spontaneously arrange to be as much far away from each other as possible, compatibly with other constraints. The 3D spatial arrangement is called *molecular geometry*: the teacher may then comment on bond angles in the different molecules and give a name to each molecular geometry.

Object of the proposed activity	Learning objectives
The GEOMAG game is used to build 3D molecular models of the same molecules examined in the previous activity	To build the concept of molecular geometry. To associate each general formula AX_mE_n (type AX_2, AX_3, AX_4, AX_2E, AX_3E and AX_2E_2) its 3D molecular geometry. To learn the rules of VSEPR theory and justify them on the basis of the students' knowledge of electrostatics

Students are organised in small groups; each group is given an adequate number of pieces (balls and sticks). The following situations are proposed (WS 23):

WS 23

1. Assemble the GEOMAG pieces in order to obtain a "model" that materially represents a molecule with the general formula AX_2 . Explain the criteria you followed.

2. Assemble the GEOMAG pieces in order to obtain a "model" that materially represents a molecule with the general formula AX_3 . Explain the criteria you followed.

3. Assemble the GEOMAG pieces in order to obtain a "model" that materially represents a molecule with the general formula AX_4 . Explain the criteria you followed.

4. Assemble the GEOMAG pieces in order to obtain a "model" that materially represents a molecule with the general formula AX_2E . Explain the criteria you followed.

5. Assemble the GEOMAG pieces in order to obtain a "model" that materially represents a molecule with the general formula AX_3E . Explain the criteria you followed.

6. Assemble the GEOMAG pieces in order to obtain a "model" that materially represents a molecule with the general formula AX_2E_2 . Explain the criteria you followed.

Students are given time to build each molecular model; the results are shared with the classroom and discussed under the teacher supervision. The teacher stimulates students to compare the structures, he tells them the rules of the VSEPR theory and show how to apply them to predict molecular geometry. The teacher stimulates the students to think about the fact that Lewis structures provide information about the connectivity between atoms in the molecule, but it lacks geometric information.

The first three molecular models of WS 23 allow discussing the linear, trigonal planar and tetrahedral geometries., the teacher ask students to predict the bond angle values typical of these geometries Based on purely geometrical arguments. The discussion of the general formula AX_nE_m allow showing that bonding electron pairs interact with two positively charged atomic kernels (those of bonded atoms), whereas the non-bonding pair interacts with a single atomic kernel. This helps rationalizing the experimental data on bond angles in molecules with non-bonding electron pairs, which deviates from ideal values. Finally, the teacher summarizes these issues in the following table:

AXE	n = X+E	Form	Disposition of electrons	Geometry	Angle	Examples
AX_2E_0	2	Linear			180	$BeCl_2$, CO_2
AX_2E_1	3	Bent			117	NO_2^- , SO_2 , O_3
AX_3E_0	3	Trigonal planar			120	BF_3 , NO_3^- , C_2H_6
AX_2E_2	4	Bent			104,5	H_2O , OF_2
AX_3E_1	4	Trigonal pyramidal			107,3	NH_3 , PCl_3
AX_4E_0	4	Tetrahedral			109,4	CH_4 , PO_4^{3-} , SO_4^{2-} , ClO_4^-

The conclusion drawn from this activity are:

- Each molecule is characterized by a specific arrangement of atoms and electron doublets in the three-dimensional space, with specific bond lengths and angles. This is called **molecular geometry**.
- **Lewis structures** show the atoms' connectivity and the distribution of valence electron pairs in molecules: they do not **provide geometrical information**;
- Molecular geometry may be predicted with the **VSEPR theory**, which focuses on the effect of electrostatic repulsion between electron pairs.

Activity 24

Goal of this WS is **to discuss the relationship between polar bonds and polar molecules**. Molecules belonging to categories AX_2 , AX_3 , etc... are examined in order to predict the position of the barycenters of positive and negative charges in the molecule. This aims at predicting whether a molecule is a permanent dipole or it is non polar.

A rigorous treatment of this issue would require introducing the vectorial quantity *dipole moment*. Our choice is to discuss polarity only from the qualitative viewpoint. A different choice would require an interdisciplinary approach, relying on physics and mathematical knowledge.

Object of the proposed activity	Learning objectives
The Lewis structures of various simple molecules are analyzed. Students are asked to make predictions on the symmetry of asymmetry of charge distribution	To build the (qualitative) notion of molecular dipole. To predict whether a substance is polar or non-polar based on its molecular geometry.

WS 24

1. Build the Lewis structures of the following substances and determine their molecular geometry by applying the VSEPR theory. Draw the structures according to their geometry.

Formula	Lewis structure	Molecular geometry
BeCl ₂		
BF ₃		
BF ₂ Cl		
CCl ₄		
CHCl ₃		
SO ₂		
NH ₃		
H ₂ O		

2. In each molecule, assess which bonds are polar and which are not. Indicates the partial charges by placing the symbols δ^+ and δ^- on each atom of the figures in column 3.
3. Based on the distribution of partial charges that you have highlighted, try to predict in which molecules the barycenters of the positive and negative charges coincide and in which they do not.

Formula	The two barycenters coincide	The two barycenters do not coincide
BeCl ₂		
BF ₃		
BF ₂ Cl		
CCl ₄		
CHCl ₃		
SO ₂		
NH ₃		
H ₂ O		

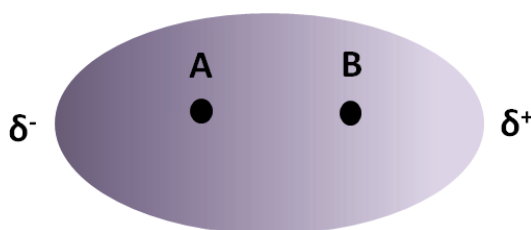
At the end of this WS, invites students to check whether these substances are classified as polar or non-polar, by looking at web sources, textbooks, etc. The results are discussed in the classroom. Some molecules turn out to be non polar, despite the presence of polar bonds. While the classroom seeks an explanation, the teacher draw the students' attention at molecular geometry. He suggests students to compare the BF₂Cl and CHCl₃

molecules (which are polar) with the BF_3 and CCl_4 molecules (which are non-polar). BF_3 and CCl_4 are symmetric: as a consequence, bond polarity is mediated to zero by the molecular symmetry. These molecules are non polar. Conversely, BF_2Cl and CHCl_3 are not symmetric: they show two polar bond and a non polar one (C-H). This implies an asymmetric distribution of the positive and negative charges in the molecule. These molecules are polar.

At the end of the activity, the teacher summarizes to the class the conclusions that have come to be shared:

- A dipole is a system wherein the barycenter of positive and negative charges do not coincide.
- Covalent bonds between elements with different electronegativity are polar, i.e. they behave as dipoles.
- A molecule may be polar (i.e. behave as a dipole) or non polar.
- A molecule containing **non-polar bonds** is **non-polar**.
- A molecule containing **polar bonds** may be **polar on non polar**, depending on its geometry. Symmetrical molecules are non polar, regardless of the presence of polar bonds.
- **The polarity of a molecule** depends on **the presence of polar bonds** and on **molecular geometry**
- **A polar substance** is made of **polar molecules**; a **non-polar substance** is made of **non-polar molecules**

Finally the teacher shows how to schematically represent a polar molecule, in order to highlight its being an electric dipole. Once again, signs δ^+ and δ^- help highlighting the asymmetrical charge distribution within the dipole:



Activity 25

The purpose of this WS is to reinforce the concepts learnt in these last activities and to exploit them for interpreting the behavior of substances A and B, from WS18.

WS 25 focuses on the fact that a dipole is a system that orients itself within an electric field. As some molecules can behave as dipoles, molecules can be sensitive to electric fields. A web application freely available at the URL: https://phet.colorado.edu/sims/html/molecule-polarity/latest/molecule-polarity_it.html is employed to this purpose, under the teacher's guide.

This simulation allows students to explore the behavior of diatomic and triatomic molecules, to vary $\Delta_{\text{Electronegativity}}$ between the atoms in the molecule, and to verify the effect of electric fields on the orientation of the resulting dipoles.

Object of the proposed activity	Learning objectives
Students use a web app to explore: • The dependence of molecular polarity on $\Delta_{\text{Electronegativity}}$ and molecular geometry • The orientation of polar molecules in the absence and presence of electric fields.	To consolidate the concept of molecular dipole and to understand its The dependence of molecular polarity on $\Delta_{\text{Electronegativity}}$ and molecular geometry To understand that electric fields affects the orientation of polar molecules in space.

Use the simulation https://phet.colorado.edu/sims/html/molecule-polarity/latest/molecule-polarity_it.html which allows you to visualize diatomic and triatomic molecular models.

Set the 'Two atoms' condition, check the three boxes under the heading 'View' and turn the 'Electric field' on.

1. Try spinning the diatom molecule. What do you notice?
2. Try to increase the electronegativity of atom B. How does the molecule's behavior change?
3. Try to increase the electronegativity of atom A so that it is greater than that of atom B. How does the molecule's behavior change?
4. Try to assign the same electronegativity to the two atoms. What do you notice?

Now set the 'Three atoms' condition, check the three boxes under the heading 'View' and turn the 'Electric field' on.

5. Try spinning the triatomic molecule. What do you notice?
6. Try to increase the electronegativity of atom B. How does the molecule's behavior change?
7. Try to exchange the electronegativities of the atoms in the molecule. What do you observe?
8. Go back to the starting situation (click on the red arrow on the right). Try to increase the A-B-C bond angle. How does the molecule's behavior change?
9. Continue increasing the A-B-C bond angle until you get a linear molecule. How does the molecule's behavior change?
10. Now increase the electronegativity of the C atom. How does the molecule's behavior change?
11. Try to attribute the same electronegativity to all three atoms. What do you notice?

Students discuss their findings and the teacher summarizes their conclusions:

- Molecular polarity depends on the presence of polar bonds and on molecular geometry.
- The highest $\Delta_{\text{Electronegativity}}$, the more polar the bond.
- Polar molecules are sensitive to external electric fields, that orientates them in space.
- Non-polar molecules are insensitive to external electric fields that cannot orientate them in space.

Activity 26

The last issue to be addressed is the interpretation of the behavior of substances A and B from WS 18 in the light of the new concepts learnt by students.

The teacher recalls that electrified glass and ebonite rods generate electric fields with opposite features. Substances A and B behaved differently:

- A was sensitive to the electric field associated with both rods
- B was completely insensitive to the electric field.

How to interpret this (macroscopic) behavior at the microscopic level? Students learnt that polar molecules are sensitive to electric fields, that can orient them in space, whereas non-polar molecules are insensitive. Does this provide a rationale for the behavior of substances A and B?

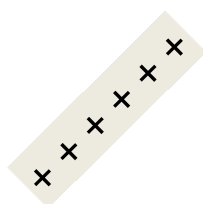
Object of the proposed activity	Learning objectives
Students are required to explain the results of the experiment done in WS 18.	To justify the behavior of ethyl alcohol and tetrachlorethylene in the presence of electric fields, at the microscopic (modelling) level.

We learnt that a polar molecule behaves like an electric dipole.

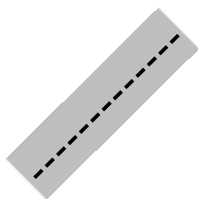
1. Given a generic molecule AB, with B more electronegative than A, represent the orientation of this molecule within the electric field below.



2. A glass rod becomes positively charged when it is electrified by rubbing. Represent the orientation of the AB molecule placed close to a glass rod.



3. An ebonite rod becomes negatively charged when electrified by rubbing. Represent the orientation of the AB molecule placed close to an ebonite rod.



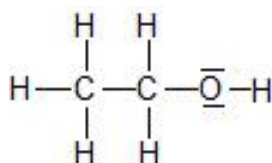
4. Consider the behavior of substance A of WS 18 (ethyl alcohol) in the presence of the glass and ebonite rods. In your opinion substance A is:
- Polar
 - Not polar
 - I do not know
 - It is not possible to answer

Justify the answer

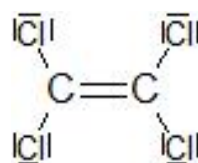
5. Consider the behavior of substance B of WS 18 (tetrachloroethylene) in the presence of the glass and ebonite rods. In your opinion substance B is:
- Polar
 - Not polar
 - I do not know
 - It is not possible to answer

Justify your answer

Examine the structural formulas of molecules A and B.



ethyl alcohol (A)



tetrachloroethylene (B)

6. In the light of what you learnt about the factors that determine the polarity of molecules, do you predict that molecule A is:
- Polar
 - Not polar
 - I do not know
 - It is not possible to answer

Justify your answer

7. In the light of what you learnt about the factors that determine the polarity of molecules do you predict that molecule B is:
- Polar
 - Not polar
 - I do not know
 - It is not possible to answer

Justify your answer

The discussion in the classroom, guided by the teacher, should lead the class to conclude that the flow of substance A was diverted by the electrified rods because substance A is made of polar molecules, behaving as electric dipoles under the action of an electric field. Conversely, the flow of substance B was not diverted because substance B is non-polar (it is made by non-polar molecules). Its molecules are non-polar (despite containing some polar bonds) due to molecular geometry.

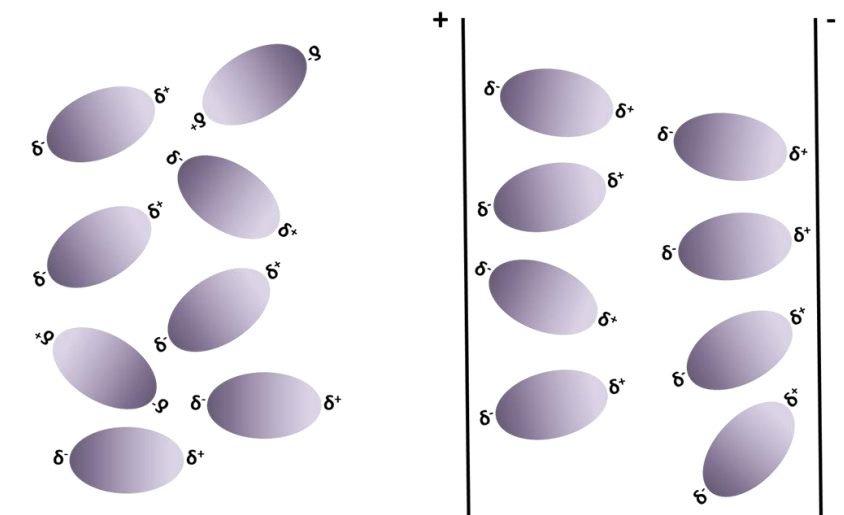


Figure 4.2 Orientation of electric dipoles in the absence and in the presence of an electric field

Students might wonder why substance A is attracted by both glass and ebonite rods, despite their being associated to electric fields with opposite orientation. The teacher may lead students to draw attention on the fact that substance A is liquid and its molecule may orient themselves according to the electric field lines.

4.4 Dipole-dipole bonding and hydrogen bridge bonding

At this stage of the teaching sequence, students are familiar with the following notion:

- Temporary dipole and London dispersion forces
- Covalent bonding
- Bond polarity
- Molecular polarity
- Permanent dipole

All the activities proposed so far insist on the nature of electrostatic¹⁴ interaction that is typical of any kind of interatomic bond.

Furthermore, the activities are ordered according to the following principle: each new concept or model that is developed and proposed to students fulfills a logical need. New concepts and models are introduced only when the students' knowledge proves insufficient or inadequate to interpret new phenomena. The sequence therefore implies the critique and evolution of interpretive models. With these premises, the topic of dipolar interactions is now addressed, based on the knowledge built in the first part of the sequence (namely, the notions of permanent and instantaneous molecular dipole).

¹⁴ Since these are electron-mediated interactions, the adjective 'electrical' is preferred to 'electrostatic' in the text. In fact, as the sequence insists on the implications of electron mobility, we believe that the term 'electrostatic' may inconsistently suggest the idea of staticity.

Activity 27

This activity aims at recalling previously learnt concepts, that help conceptualizing dipole-dipole interactions (WS 28).

Object of the proposed activity	Learning objectives
The HCl molecule is drawn and students are asked to apply the previously learnt criteria to determine whether the molecule is polar or non-polar.	To consolidate the concept of molecular dipole and the way to represent it through symbolic language.

WS 27

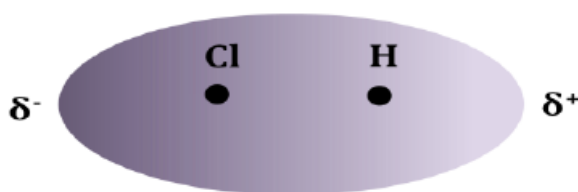
1. Write the formula of hydrogen chloride and build its Lewis structure.
2. Write the electronegativity values of chlorine and hydrogen (you can find them in the WS 20 table)
Hydrogen
Chlorine
3. Based on the data available and the criteria you have learnt, do you think that the HCl molecule is:
 - polar;
 - apolar;
 - it is not possible to answer;
 - I can not answer.

Justify your choice.

4. Represent the HCl molecule highlighting whether the barycenters of the positive and negative charges coincide or not (for this purpose you can use the symbols δ^+ and δ^- , where applicable)

Students use the electronegativity table values and apply the above-discussed criteria to assess HCl polarity. HCl is a polar molecule, with the barycenter of negative charges close to the chlorine atom. This can be represented by symbols δ^+ e δ^- put close to H and Cl, respectively.

Students, who are already familiar with these pictures from WS 24, are expected to draw images like this:



The classroom is expected to agree on the fact that HCl is made of permanent dipoles that interact with each other through electric interactions: this situation is similar to that described for instantaneous dipoles (He atoms and H₂ molecules) met in previous activities.

Activity 28

This activity aims at helping students realise the physical consequences of the presence of bonds between dipolar molecules. In analogy to the case of temporary dipoles, the extent of the interaction between molecules determines the physical state of the substance at a given temperature and pressure. Furthermore, this WS resume the concept that dipolar interactions do not involve pairs of molecules: they occur between all molecules of a given polar substance (even though the extent of the interaction decreases with distance).

Object of the proposed activity	Learning objectives
Students are required to draw particle representations of hydrogen chloride in the solid, liquid and gaseous state.	To consolidate the concept that electrical interactions occur between HCl molecules . These intermolecular bonds are called dipole-dipole bonds.
The boiling and melting temperatures of two polar substances are compared.	To understanding the relationship between the extent of dipole-dipole bonds and the physical state of a given substance at a fixed temperature and pressure.

Experimental data show that, at atmospheric pressure, the substance HCl is in the solid state below -114.22° C and in the gaseous state above -85.05° C.

- In your opinion, are there bonds between HCl molecules?
 - yes, there are;
 - no, there aren't;
 - it is not possible to answer;
 - I can not answer.
- Which of the following statements are correct and which are not? Answer by choosing between the True or False

	TRUE	FALSE
a. HCl molecules do not interact with each other at any T and P		
b. HCl molecules are electric dipoles		
c. There are no bonds between HCl molecules		
d. HCl molecules interact through electric interactions;		
e. Electric dipoles interact with each other		

- Represent substance hydrogen chloride at the particle level, in the **solid** state, keeping in mind that each molecule of the substance HCl is an electric dipole. Justify what you have drawn.
- Represent substance hydrogen chloride at the particle level, in the **liquid** state, keeping in mind that each molecule of the substance HCl is an electric dipole. Justify what you have drawn.
- Represent substance hydrogen chloride at the particle level, in the **gaseous** state, keeping in mind that each molecule of the substance HCl is an electric dipole. Justify what you have drawn.

Consider the following table, which compares some physical data of two polar substances:

	melting temperature (°C)	boiling temperature (°C)
HCl	-114,22	-85,05
SO ₂	-75,5	-10,0

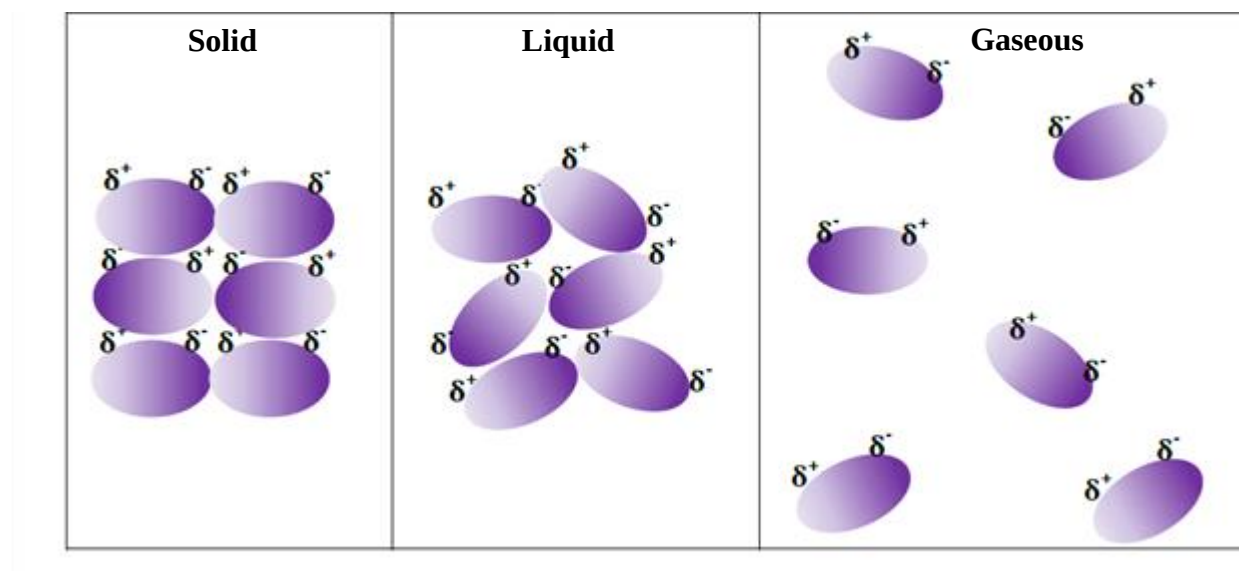
- In the light of the experimental data and of what you have learnt so far, can you predict which of these substances is more polar? Justify your answer.

- In the light of the experimental data and of what you have learnt so far, can you predict in which substance the binding force between molecules is higher? Justify your answer

Questions 1 and 2 aim at recalling that a (covalent) substance can be modeled as a set of interacting molecules, i.e. there are electrical bonds between them. **The substance could not subsist without intermolecular interactions.**

The particle representations of hydrogen chloride in three physical states helps 'visualising' the previous statement; it also highlights the fact that permanent dipoles 'orient' each other, as the positive poles of each molecule interacts preferentially with the negative pole of another molecule.

The type of representations expected in response to questions 3, 4 and 5 are as follows:



Students' drawings are examined by the teacher and discussed in the classroom. The teacher summarises the following conclusions:

- Molecules of polar substances can be represented as **electric dipoles**.
- They interact with each other through **electrical bonds**.
- **The extent of the interaction** determines whether the substance is **solid, liquid or gaseous at room temperature and pressure**.
- The extent of the interaction decreases with increasing temperature.

Activity 29

This activity compares the extent of dipolar interaction and London forces in isoelectronic systems. London dispersion forces have been shown to depend on i) the number of electrons involved; ii) their distribution in space; iii) the distribution of nuclear charges in the system.

In this activity, two isoelectronic (polar and non-polar) systems are compared and their boiling temperatures are discussed.

Object of the proposed activity	Learning objectives
Students are asked to compare the boiling temperatures of two substances (non-polar and polar) substances, whose molecules are isoelectronic.	To assess the relative extent of dipolar interactions and London dispersion forces (in isoelectronic systems).

Look at the data in the table below:

Substance	F ₂	HCl
Total number of electrons	18	18
Boiling temperature (° C)	-188	-84,2
Type of bond	Non-polar Covalent	Polar Covalent

1. Based on what you learnt so far, what kind of bond exists BETWEEN F₂ molecules? Justify your answer.

2. Based on what you learnt so far, what kind of bond exists BETWEEN HCl molecules? Justify your answer

You learnt (WS 5-11) that the extent of the interaction between instantaneous dipoles depends on: i) the number of electrons involved; ii) their distribution in space; iii) the distribution of nuclear charges in the system. Here we have two molecules with the same number of electrons: one is an instantaneous dipole and the other a permanent dipole.

3. In your opinion, which bonds need more energy to be broken? Those between F₂ molecules or those between HCl molecules? Justify your answer.

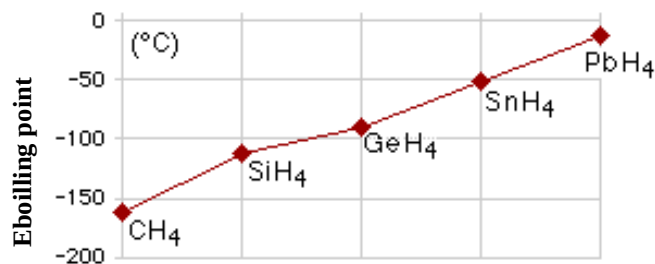
4. In your opinion, which of the two substances displays the stronger bonds between molecules? Justify your answer.

F₂ and HCl are isoelectronic, a condition that allows comparing the strength of their intermolecular interactions, all other things being equal. Students' answers are shared in the classroom and the discussion focuses on questions 3 and 4. HCl boils at higher temperature than F₂. This means that intermolecular interactions are stronger in HCl (which is polar) as compared to F₂ (which is non polar).

Activity 30

This activity is preparatory to discuss the H bridge bond.

Look at the following graph which shows the boiling temperatures of the hydrides of the elements of the fourth group of the periodic table.



1. In your opinion, the molecules of the hydrides of the fourth group are:

- polar;
- non-polar;
- I can not answer.
- it is not possible to answer.

Justify your choice.

2. Based on what you learnt so far, what type of bond is present between the molecules of these hydrides? Justify your answer

3. How do you explain the increase of boiling temperatures from CH₄ to PbH₄?

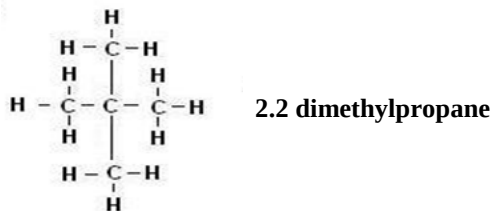
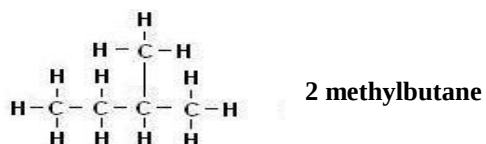
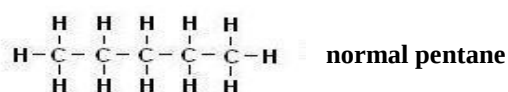
The classroom discussion should lead students to share the conclusion that these substances are made up of molecules with general formula AX₄, which are perfectly symmetrical. Therefore, they are non-polar and behave like instantaneous dipoles, interacting by London dispersion forces. Boiling temperatures are an index of the extent of these interactions. While shifting from CH₄ to PbX₄, there is an increase of: i) number of electrons in the molecule; ii) molecular volume; iii) nuclear charge of A. This may explain the increase in the extent of London dispersion forces along the series, witnessed by the increase of boiling temperatures.

Activity 31

Students already know that the extent of London forces is affected by the distribution of electron in space, which relates to molecular volume and surface area. However, so far they always compared compounds in homologous series. It is now matter of taking into consideration some structural isomers of simple hydrocarbons, characterized by very different shapes (and therefore contact surfaces). WS 31 proposes to compare three structural isomers, whose different boiling temperatures depend solely on molecular volume and shape.

Object of the proposed activity	Learning objectives
The boiling temperatures of three structural are compared.	To understand that the extent of London forces is affected by molecular shape, volume, and surface area.

In a chemistry textbook, the following three Lewis formulas are represented, which refer to the molecules of three different substances.



1. After looking at the Lewis structures of the three molecules, complete the following table:

Substances	Normal pentane	2 methylbutane	2,2-dimethylpropane
Total number of C atoms			
Total number of H atoms			
Total number of electrons			
Boiling temperature (°C)	36	28	10
Type of intra-molecular bond			
Type of inter-molecular bond			

2. In your opinion, what differentiates the three molecules?
-
3. Take the stick-and-ball models of normal pentane and 2,2-dimethylpropane available in the classroom. Try:
- To take three molecules of normal pentane close together;
 - To take three molecules of 2,2-dimethylpropane close together.

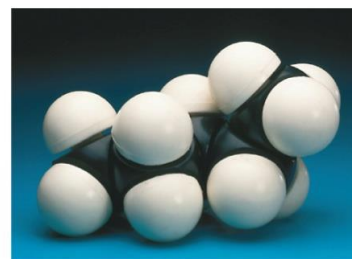
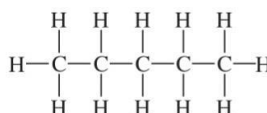
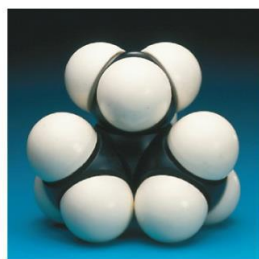
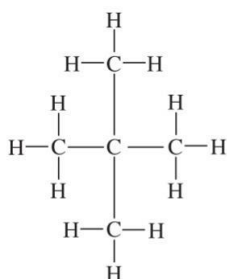
In your opinion, in which case the contact surfaces between molecules are more extended?

- In the case of normal pentane
- In the case of 2,2-dimethylpropane
- It is not possible to answer
- I can not answer

Justify your answer

4. In the light of what you learnt so far, how do you explain the trend of the boiling temperatures of these three substances?
-

The overall discussion, led by the teacher, focuses on the fact that these molecules display the same number of C and H atoms; in addition, they are isoelectronic. All of them are non polar and interact through London forces. However, their atoms are differently connected (see Lewis formulas) and their molecular geometry is different. Consequently, the shape of these molecules is different. To help students visualising these aspects, it is possible to molecular models or 3D simulations (e.g. Rasmol) are used:



By handing molecular models, students realise that the contact area is larger in normal-pentane as compared to neopentane. Based on their knowledge on London forces, students will easily predict that London interactions are stronger in normal pentane, as witnessed by its higher boiling temperature.

Activity 32

This further activity focuses on the fact that London's forces are present in all substances, although their 'relative weight' can vary greatly as compared to other intermolecular interactions. The homologous series halogen hydrides (excluding HF) and their boiling and melting temperatures are taken into consideration. Students learnt that these substances exhibit polar covalent bonds, hence their molecules are permanent dipoles and display dipolar interactions. However, the trend of boiling and melting temperatures is inconsistent with the presence of just dipolar interactions. This inconsistency can be exploited to show that London forces concur to intermolecular interactions in any molecular substance. Therefore, the trend of boiling and melting temperature trends can be interpreted as the result of two phenomena (dipolar interactions and London forces) whose relative weight changes from substance to substance.

Object of the proposed activity	Learning objectives
Students are asked to compare experimental data of the homologous series of halogen hydrides and to interpret them in the light of their previous knowledge.	To understand that London dispersion forces are not peculiar of non-polar substances. To understand that the physical properties of substances may be interpreted as the result of various kinds of molecular interactions, whose relative extent varies from substance to substance.

Look at the following table:

Substance	HCl	HBr	HI
Melting temperature (°C)	-114,22	-87	-50,8
Boiling temperature (°C)	- 85,05	-67	-35,36
Δ electronegativity between the two elements	0,85	0,7	0,49
Atomic radius of the two elements involved (pm)	H 37 Cl 99	H 37 Br 114	H 37 I 133
Type of intra-molecular bond			
Number of f electrons in the molecule			

- Complete the table based on what you learnt so far about chemical bonds
- Based on the electronegativity difference, which of the three substances is more polar and which is less polar? Justify the answer

- Based on the bond models you learnt so far, the trend of the boiling and melting temperatures in the three substances is:
 - As you would expecte
 - Different from what you expected
 - It is not possible to answer
 - I can not answer

Justify your answer

- Can the interaction between molecules of the same substance be determined by several different mechanisms?
 - yes;
 - no
 - it is not possible to answer
 - I can not answer

Justify your choice.

In previous activities, students learned that polar molecules interact through dipole-dipole bonds and that - all boundary conditions being equal - this type of bond is stronger than London's dispersion forces (i.e. more energy is required to break it). This statement seems disproved by the trend of boiling and melting temperatures of these three hydrides. Is dipole-dipole intermolecular bond model therefore disproved? Should it be replaced by another model? Should it be modified? The teacher draws students' attention to the specification 'with the same boundary conditions'. These three are not isoelectronic and exhibit different

molecular volumes (due to the distinct atomic radii of halogens hydrides). This makes these systems not directly comparable. The discussion of students' answers, led by the teacher, should lead students to reflect on the fact that London forces are known to increase with increasing electron number and molecular volume. This condition is met along this series: hence these molecules are likely to exhibit London interactions, whose extent increases along the series. Concurrently, bond polarity decreases along the series, from HCl to HI: hence, these molecules are polar, but the extent of their polarity decreases along the series. The teacher suggests that **these three substances exhibit two types of interactions (dipole-dipole bonds and London dispersion forces) that exhibit opposite trends**. The extent of dipole-dipole bonds decreases along the series, whereas the extent of London forces increases: the boiling and melting values are determined by the relative extent of these interactions. For example, in HI dipole-dipole bonds are much weaker than London dispersion forces as compared to HCl. This hypothesis is consistent with the trend of the chemical-physical data and **can be generalized to other substances**. In conclusion, **London dispersion forces are typical of any chemical species, although their extent may be negligible as compared to other intermolecular interactions**.

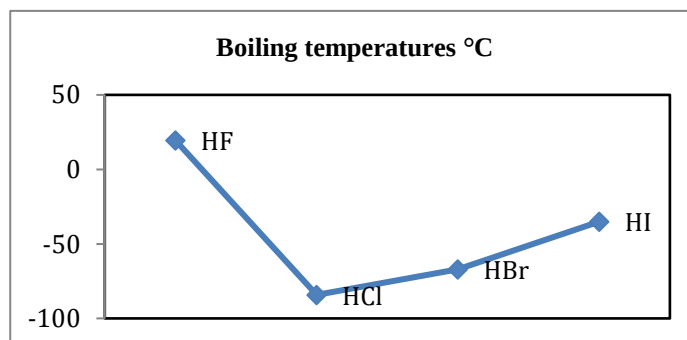
Activity 33

The last type of dipolar interaction that remains to be treated is the hydrogen bridge. Since it is a special case of dipolar bond, it has to be tackled after discussing dipolar interactions. Its peculiarities are related to the high $\Delta_{\text{electronegativity}}$ between the atoms involved in this kind of bonding, the small size of hydrogen atoms, its directionality.

To introduce this type of bond, students are asked to examine the trend of boiling temperatures of halogen hydrides in the light of their previous knowledge. The inconsistent behavior of HF is then discussed.

Object of the proposed activity	Learning objectives
Students are asked to examine the trend of boiling temperatures of halogen hydrides and to analyse the anomalous behaviour of HF.	To understand that the anomalous behavior of HF is correlated to the high electronegativity of F with respect to H and the small size of both the atoms of F and H, which enhances dipole-dipole interactions.

Look at the trend of the boiling temperatures of the halogen hydrides.



In WS 32 you examined the boiling and melting temperatures trends of substances HCl, HBr and HI and you justified them in terms of bonds between permanent dipoles and/or instantaneous dipoles.

- Based on the data in the graph, which one of the following statements is correct, in your opinion?
 - The bonds between HI molecules are stronger than those between HCl molecules
 - More energy is required to loosen the bonds between HCl molecules than those between HBr molecules
 - The bonds between HF molecules are stronger than those between HBr molecules
 - More energy is required to loosen the bonds between HCl molecules than those between HF molecules
- In the light of what you learnt so far, how can you explain the behavior of HF with respect to other hydrides? Look at these hypothesis:
 - In HF there is a bond of a completely different nature than those found in the other three substances
 - In HF the dipole-dipole bonds prevail over the bonds between instantaneous dipoles
 - In HF bonds between instantaneous dipoles prevail over dipole-dipole bonds
 - I don't know
 - It is not possible to answer

Justify your choice

- Complete the table below by searching the missing data in the Periodic Table:

Substances	HF	HCl	HBr	HI
Δ electronegativity between the two elements				
Atomic radius of the two elements present in the molecule (pm)	H 37 F 64	H 37 Cl 99	H 37 Br 114	H 37 I 133
Total numbers of electrons present in the molecule				

- Based on the data in the table, sort these substances in order of increasing polarity. Justify your answer.
-

5. Sort the elements of the table according to increasing atomic radii (and therefore atomic volumes).

6. Which element displays the smallest atomic radius?

7. Which halogen displays the smallest atomic radius?

8. Based on the data in the table, which is the more polar bond between H-F and H-Cl? Justify your answer.

9. Based on the data in the table, do you expect that:

- Dipole-dipole bonds between HI molecules are stronger than those between HF molecules
- Dipole-dipole bonds between HF molecules are stronger than those between HCl molecules
- Dipole-dipole bonds between HCl molecules are stronger than those between HF molecules
- Dipole-dipole bonds between HBr molecules are stronger than those between HI molecules

Justify your choice.

10. Graphically represents the interaction between HF molecules in the gaseous state, and the interaction between HCl molecules in the gaseous state. Highlight molecules's polarity by using the symbols δ^+ and δ^- and pay attention to the different size of H, F and Cl atoms.

HF in the gaseous state

HCl in the gaseous state

Question 1 focuses on the relationship between boiling temperatures and the extent of inter-molecular bonds. Question 2 aims at connecting the previous issue to the conclusions of activity 32: HF has an apparently anomalous behavior. However, this behavior can be rationalized by considering that, in this molecule, dipolar bonds prevail over London interactions. The goal of this question is to avoid introducing the H bridge bond as a completely new type of bond and to discuss it as a special case of dipolar bond. The reason for this peculiarity need to be explored: Questions 3 and 4 focus on the strong polarization of H-F covalent bonds as compared to the others substances. Questions 5-8 aim at rationalizing this unusual polarisation, based on the data in the table: fluorine is the most electronegative element and also the smallest of the halogens, H is also very small.

Question 9 takes up question 1 from a different perspective: in fact, question 1 mentions macroscopic data (boiling temperatures), whereas question 9 mentions data deriving from microscopic models.

Question 10 aims at making students visualize the two microscopic systems HF and HCl and to highlight the different molecular size.

The discussion in the classroom is expected to lead to the following shared conclusions:

- The boiling temperatures of the halogen hydrides mirror the extent of intermolecular interactions.

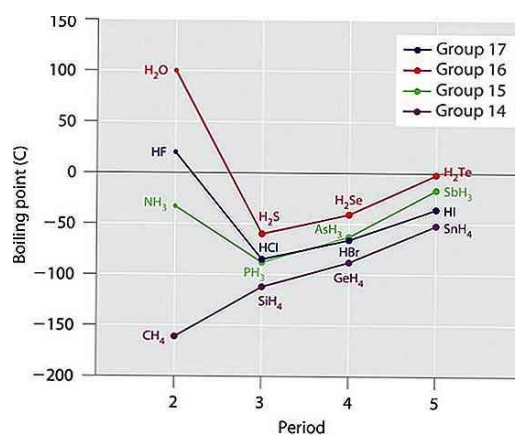
- In HCl, HBr and HI, the extent of London forces is comparable to the extent of dipolar interactions. In HF, the reverse occurs.
- The H-F bond is strongly polarized due to the small size of the H and F atoms and the high $\Delta_{\text{electronegativity}}$ between them.

Activity 34

Activity 34 aims to generalize the conclusions of the previous activity to other substances that exhibit a behavior similar to HF. The trend of boiling temperatures of various homologous series of hydrides is interpreted according to the same interpretive criteria already applied to HF. At the end, the teacher comments on the peculiarities of dipolar interactions in substances like ammonia, water or hydrogen fluoride, all of which contain very electronegative atoms bonded to the small hydrogen atom (i.e. they exhibit H-X type covalent bonds).

Object of the proposed activity	Learning objectives
Students are asked to examine the trend of boiling temperatures of the hydrides of group 4, 5, 6 and 7 elements and to analyse their trend.	To understand that the anomalous behavior of HF, H₂O and NH₃ can be interpreted in a similar way. To introduce the H bridge bond as a peculiar kind of dipolar interaction, typical of substances with strongly electronegative atoms bonded to the small hydrogen atom (H-X type covalent bonds).

Look at the trend of the boiling temperatures of the hydrides of the elements of the fourth, fifth, sixth and seventh group of the Periodic Table:



1. Is the behavior of H-F we studied in the previous WS shared by other substances?

- yes, it is;
- no, it isn't;
- I cannot answer.

If so, by which ones?

2. Look at the trend of the boiling temperatures of the hydrides of the sixth group. Do you see analogies with the hydrides of the seventh group?

- yes, I do;
- No, I don't;
- I cannot answer.

If so, which ones?

3. Look at the trend of the boiling temperatures of the hydrides of the fifth group. Do you see analogies with the hydrides of the seventh group?

- yes, I do;
- No, I don't;
- I cannot answer.

If so, which ones?

4. Look at the trend of the boiling temperatures of the hydrides of the fourth group. Do you see analogies with the hydrides of the seventh group?

- yes, I do;
- No, I don't;
- I cannot answer.

If so, which ones?

5. In your opinion, the substances that, in each group, do not follow a linear trend are:

- more polar than other substances of the same series
- less polar than other substances of the same series
- it is not possible to answer
- I cannot answer

Justify your answer.

6. Based on the data reported in the graph, which one of the following statements is correct?

- a. The bonds between NH_3 molecules are stronger than those between PH_3 molecules
- b. More energy is required to loosen the bonds between H_2S molecules than those between H_2O molecules
- c. Less energy is required to loosen the bonds between H_2O molecules than those between HF molecules
- d. The bonds between the CH_4 molecules are weaker than the bonds between the NH_3 molecules

Justify your answer.

7. In the light of what you learnt in activities 32 and 33, can you interpret the behavior of the substances reported in the WS 34A graph?

8. Provide a graphical representation of the bond between molecules HF , NH_3 , H_2O and CH_4 molecules in the gaseous state and highlight molecule's polarity by using symbols δ^+ e δ^- , if appropriate.

HF	NH_3	H_2O	CH_4

Questions 1-4 aim at highlighting the anomalous behavior of HF , NH_3 , H_2O in groups 5, 6 and 7, whereas group 4 follows a linear trend.

Question 5 focuses on the polarity of substances that deviates from linearity. The teacher leads the classroom to realise that H-X bonds are found in these substance, with X strongly electronegative.

Question 6 focuses on energetic aspects: students are expected to interpret high boiling temperatures as sign of the presence of strong inter-molecular bonds. Hence, substances deviating from linearity are characterized by strong inter-molecular bonds.

Questions 7 and 8 allow assessing the students' ability to use the knowledge and concepts developed in previous activities.

All questions are discussed in the classroom and the teacher summarise the conclusions:

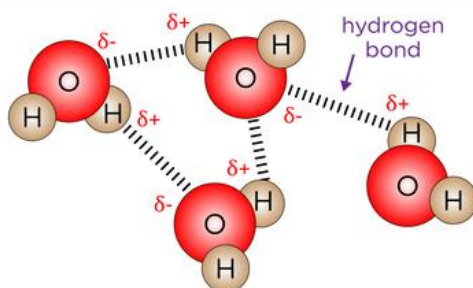
- Within each homologous series, oxygen, fluorine and nitrogen are the most electronegative elements; their size is smaller as compared to the other elements of the same series.
- All substances that deviate from linearity contain strongly polarised H-X bonds, with X strongly electronegative and H rather electropositive. Both X and H atoms exhibit a small size.
- As substances HF, NH₃, H₂O are the most polar within each homologous series, the extent of their dipolar interaction is greater as compared to their homologous substances. Hence, the extent of London dispersion forces is negligible.
- The C-H bond is not polarized. Consequently, methane molecules are instantaneous dipoles and exhibit only London dispersion forces, just like their homologous substances in the series: this explains the linear trend of the 4th group.

After examining the drawings of question 8, the teacher points out that all substances with H-X covalent bonds (with X strongly electronegative) exhibit peculiar dipolar interactions, mediated by the H atom, which act as a 'bridge' between two molecules, due to its small size. This kind of bond is called **hydrogen bridge**.

Students often mix up hydrogen bonds and H-X intramolecular bond. The teacher may ask further questions, aimed at discussing and clarifying this aspect:

- Do you think it takes more energy to remove two water molecules bonded through a hydrogen bridge or to take hydrogen and oxygen atoms apart from a water molecule?
- In your opinion, may the hydrogen bridge bond be represented by a stick, in analogy to covalent bonds?

The discussion in the classroom should help clarifying that H-bonds are weaker than covalent bonds, as the former is intermolecular, whereas the latter is intramolecular. The 'stick' representing covalent bonds stays for a shared electron pair. So hydrogen bonds need a distinct symbol: they are generally represented by dashed lines, as shown in the figure 4.3:



4.3 Representation of the hydrogen bridge bond between water molecules

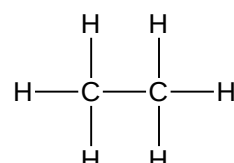
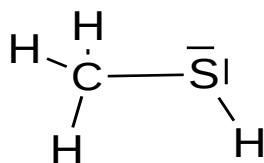
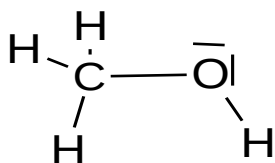
Activity 34 bis (optional)

Contextualization activity: where can H-bonds be found in nature?

Aim of this activity is to discuss the relation between some chemico-physical properties of substances and the presence of the hydrogen bridges. The teacher exploits WS 35 to ask students some questions. Hydrogen bridges may help justifying various properties such as: physical state at a given pressure and temperature, miscibility and solubility in specific solvents, viscosity. Furthermore, hydrogen bridges allow proteins to structure in space, they are perturbed by some hair treatments and are responsible for the hydrating effects of substances found in anti-aging cosmetics.

Object of the proposed activity	Learning objectives
Students are asked to answer questions that contextualize the hydrogen bridge bond in real systems.	To consolidate students' awareness relation between some chemico-physical properties of substances and the presence of the hydrogen bridges. To identify phenomena of daily life in which hydrogen bridge bonds come into play.

Look at the Lewis structures of the following substances:

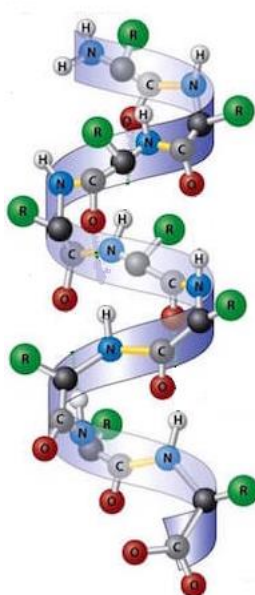


Methanol (CH_3OH) is liquid at room temperature and pressure; it boils at 65°C .

Metanthiol (CH_3SH) boils at 6°C ; therefore, it is a gas at room temperature and pressure.

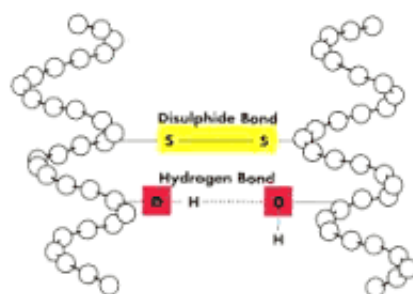
Ethane (CH_3CH_3) is also a gas at room temperature and pressure; in fact, it boils at -89°C .

1. Could you justify the differences between the boiling temperatures of these three substances?
2. Look carefully at this representation of the α -helix of a protein:



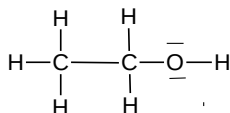
The alpha-helix is held together by hydrogen bridge bonds, which were not represented in this image. Could you identify their location? Indicate with circles drawn on the figure.

3. The following image represents the chemical bonds between two α -helices in hair keratin:

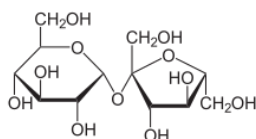


In your opinion, what happens when the hair is straightened or when a styling is done? Why is this effect temporary?

4. Reconsider Table 4.1. You will notice that ethanol (whose Lewis's formula is shown below) is soluble in water, otherwise there would be no alcoholic beverages. In your opinion, why is ethanol very soluble in water? Reply by accompanying your answer with graphical representations.

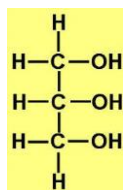


5. Look at this representation of the structure of sucrose, i.e. common sugar:



In your opinion, why is sucrose very soluble in water?

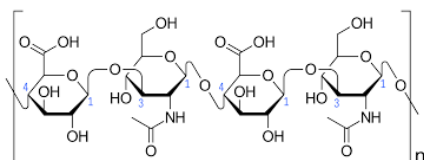
6. At room temperature and pressure, glycerol is a rather viscous liquid. Viscosity represents the resistance of a fluid to flow. Look at the representation of the structure of glycerol (commonly called glycerin).



- In your opinion, why is it a rather viscous liquid at room temperature?
-

- In your opinion, why does the liquid become less viscous as temperature increases?
-

7. Hyaluronic acid is a polysaccharide widely used in moisturizing cosmetics. Look at its structural formula and try to explain why it has moisturizing properties for the skin



Students' answers are discussed in the classroom and the teacher summarizes the outcome of the discussion:

- Hydrogen bonding may affect the physical state of some substances.
- Hydrogen bonding may affect some substances' miscibility or solubility in water
- Hydrogen bonding is responsible for the viscosity of liquids such as glycerol: when temperature increases, glycerol viscosity decreases due to the loosening of hydrogen bridges
- Hydrogen bonding is responsible for the establishment of protein secondary structures, such as the α -helix.
- Hydrogen bonding is perturbed in hair styling, as this practice involves the temporary breaking of hydrogen bridges. The transient character of this treatment is due to the low amount of energy involved in hydrogen bonding, that ease the re-establishment of these bonds in hairs.

4.5 Ionic bonding model

The activities developed in the sequence up to this point allowed modelling the (pure and polar) covalent bond, which accounts for the properties of molecular substances. By looking at the properties of ionic substances (class A in Table 4.1), it is immediately evident that the covalent bonding model cannot interpret properties such as the electrical conductivity of NaCl in the molten state or in solution. This model is unfit to deal with ionic substances and a new bonding model needs to be developed. This aim can be achieved through the critique and the evolution of the covalent bonding model, based on the following logical steps:

- i) ionic compounds, unlike covalent substances, conduct electricity in the molten state or in water solution, whereas they don't in the solid state: therefore they must contain charges that are mobile only in the liquid state or in solution; the most likely candidates are ions;
- ii) the application of the Lewis model allows highlighting that, for some elements (typically, alkaline and alkaline earth metals and non-metals), the condition that has been identified as stable (i.e. to exhibit full outermost electron shell) involves electron transfer between atoms. This process results in the formation of ions. This process can be seen as a condition of extreme bond polarity, thus emphasizing the continuity with the covalent bonding model. The ionic bonding model can therefore be seen as an evolution of the covalent one, since its basic logical foundations (energetic factors, stability of full shell configurations) are the same;
- iii) A relevant logical implication of ions' formation is the adirectional character of the resulting bonds, due to the fact that the electric field associated with each single ion is isotropic. Therefore, there is no need to hypothesize a preferential interaction between couples of atoms, as in covalent systems. The concept of *molecule* is here replaced by the *lattice*.

From the theoretical point of view, the ionic bonding model is inspired to the theory of the German physicist Walther Kossel (1916). According to Kossel, ion formation can be explained by considering that, given two distinct atoms A and B, the core of atom B might attract the outershell electrons of A more strongly than the core of atom A: this induces an electron transfer from A to the 'zone of influence' of core B, with the consequent formation of ions with opposite charges.

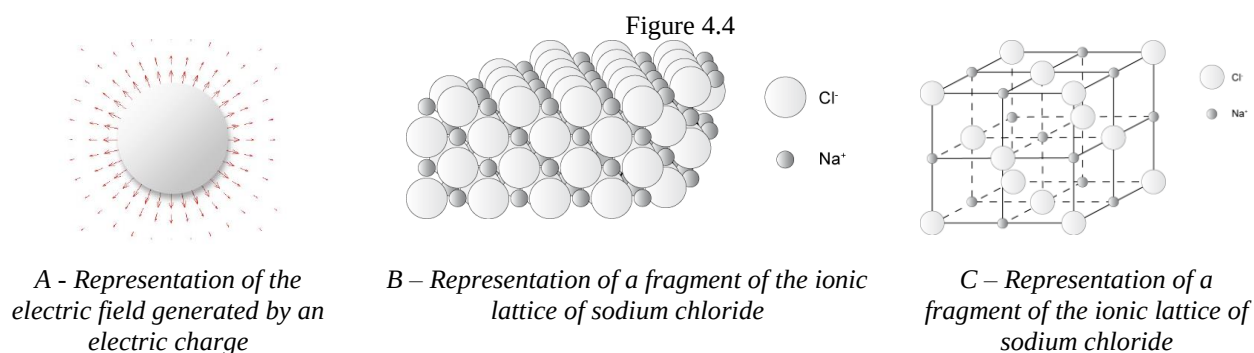
The connection with the covalent bonding model can therefore be done in the following terms:

Let's take a sodium atom and a chlorine atom, whose electronegativity difference is very high: $\Delta_{\text{electronegativity}} = 3.0 (\text{Cl}) - 0.9 (\text{Na}) = 2.1$. The application of the covalent bonding model should result in the formation of a polar bond. However, Lewis structures immediately highlight that - in this case - there is no way to attain a

stable electronic configuration by electron sharing. The only possibility to get atoms with full outermost electron shells is electron transfer.

The electronegativity difference can be read in Kossel's terms: the attraction of the Chlorine core towards the electron of the Sodium outer shell is stronger as compared to the Sodium core. Consequently, the electron of Sodium outer shell spends most time next to the Chlorine core. Chlorine therefore acquires a permanent excess of negative charge: it becomes a negative ion, an anion; conversely, Sodium exhibits an excess of positive charge: it becomes a positive ion, a cation. Anions and cations are held together by an electrical force that obeys Coulomb's law, i.e. Coulombian attraction (see Activity 4).

May we say that ionic substances are made of 'ionic molecules'? Coulomb's law disproves it. An ion can be represented as a sphere with an electric charge. Each electric charge placed in space generates an electric field around itself whose symmetry is spherical. In other words, an electric charge modifies the properties of the surrounding space in such a way that any other electric charge placed nearby is affected by the electric field regardless of its spatial position (Figure 4.4): there isn't any directional preference. It follows that an ionic compound cannot be made of molecules, since ionic bonds are non-directional.



The resulting system, made by anions and cations, is characterized by the balance of attractive and repulsive interactions between charges: this balance condition corresponds to a potential energy minimum, in analogy to the issues discussed in activity 13. Ions aggregate into three-dimensional structures called *ionic lattices* (usually represented as in Figure 4.4 B or 4.4 C) that explain the formation of solid crystals observed at the macroscopic level. It is therefore the balance of attractions and repulsions that determines the mutual arrangement of ions, i.e. the number of positive ions that are next to the negative ones, and vice versa.

The spatial arrangement of the ions depends on two factors: i) the charge and ii) the size of each ion. The comparison between the structures of two ionic substances (sodium chloride and cesium chloride, Figure 4.5) may help exemplifying this topic.

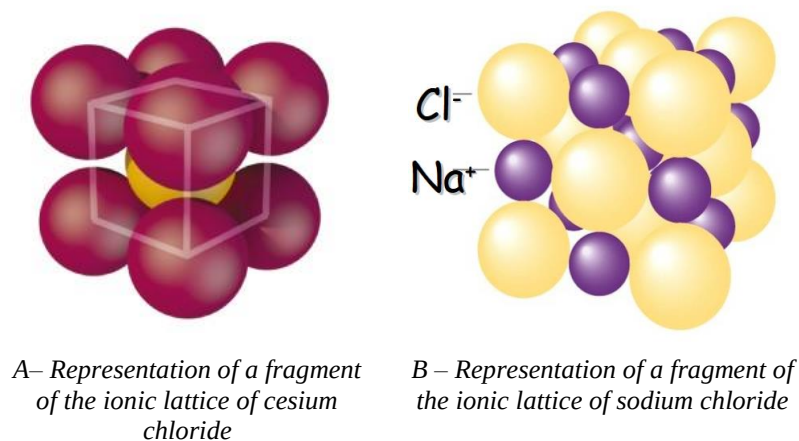


Figure 4.5 Representations of two different ionic lattices

Figure 4.5 shows how coordination numbers may differ in distinct substances, despite the presence of equally charged ions: in fact, distinct ionic radii (Na^+ 102 pm; Cs^+ 169 pm; Cl^- 181 pm) determine different packaging. The last problem to be faced is of a lexical nature: ionic substances are designated by formulas such as NaCl or CaF_2 , that specify:

- i) The type of elements in the substance
- ii) The stoichiometric ratio between positive and negative ions, resulting in electrically neutral species

These formulas do not designate molecules, but 'unit-formulas', that is a symbolic entity that does not correspond to any composite material particle. This issue needs to be discussed with students.

Ionic bonding model accounts for the following macroscopic properties of ionic substances:

- They are solid at room temperature.
- they are not electric conductors in the solid state
- they are electric conductors in the liquid (molten) state
- They are water soluble (thanks to ion-dipole interactions).
- they are electric conductors in aqueous solution.
- Their melting and boiling points are high (high bonding energies).
- They are fragile (if a mechanical stress leads positive (or negative) ions close to each other, charge repulsions prevail and the material body fragments) (Figure 4.6).

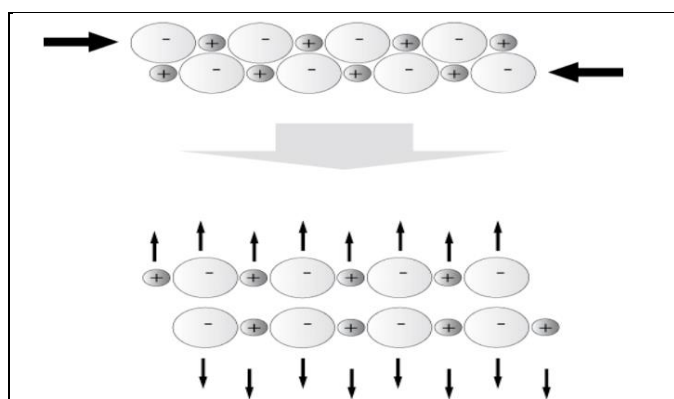
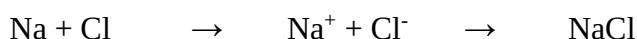


Figure 4.6 - Fragility of ionic solids

Our approach to the ionic bond takes into account the most widespread misconceptions reported in the literature, and in particular the so-called Molecular Framework (Taber, 1997), widely discussed in §2.5 of this thesis.

In order to do so, we exploit the comparison between the macroscopic properties of ionic and molecular compounds. This approach also complies with the idea that material reality comes first, and explicative models follow. In fact, symbolic representations like this one:



that are often found in textbooks for introducing ionic bonding, may lead students to believe that the ionic bond occurs between pairs of ions and generates molecules.

Activity 35

Students are asked to look at the macroscopic properties of the substances, summarized in Table 4.1. The questions of WS35 focus on electrical conductivity of substances and stimulate the comparison between insulators (such as sucrose) and conductors (such as sodium chloride), at the particle level.

Object of the proposed activity	Learning objectives
The conductive or insulating properties of some covalent or ionic substances are compared.	To highlight the different behavior of ionic and covalent substances as regards to electrical conductivity.

WS 35

Reconsider the data collected in Table 4.1.

1. Ethyl alcohol (liquid substance at room temperature and pressure) is:

- conductor of electricity;
- insulator;
- other;
- I can't answer.

Justify your choice:

2. Sucrose (solid substance at room temperature and pressure) is:

- conductor of electricity;
- insulator;
- other;
- I can't answer.

Justify your choice:

3. Sodium chloride (solid substance at room temperature and pressure) is:

- conductor of electricity;
- insulator;
- other;
- I can't answer.

Justify your choice:

Students are expected to justify their choices by making explicit reference to the experimental data reported in Table 4.1. It should be stressed that these three substances have been assigned to different sets, in the table. Some students might propose interpretations that exclude the presence of electrical charges. The teacher records the different ideas and invites the classroom to compile worksheet 36.

Activity 36

The same questions are asked again, but they refer to the same substances in water solution.

Object of the proposed activity	Learning objectives
The conductive or insulating properties of some covalent or ionic substances in aqueous solution are compared.	To highlight the different behavior of ionic and covalent substances in water solution as regards to electrical conductivity. To connect electrical conductivity to the presence of mobile electrical charges.

Reconsider the data collected in Table 4.1.

1. An aqueous solution of ethyl alcohol is:

- conductor of electricity;
- insulator;
- other;
- I can't answer.

Justify your choice:

2. An aqueous solution of sucrose is:

- conductor of electricity;
- insulator;
- other;
- I can't answer.

Justify your choice:

3. An aqueous solution of sodium chloride is:

- conductor of electricity;
- insulator;
- other;
- I can't answer.

Justify your choice:

The comparison of students' answers to the questions of WS 35 and 36 should highlight the peculiar behavior of sodium chloride, that behaves as electrical conductor only in aqueous solution, whereas the other substances are insulators. The teacher will point out that NaCl is a conductor also in the liquid state (molten salt), whereas the other two substances are not.

From the physics course, students should have developed the concept that electrical conduction is only possible in the presence of **free electrical charges**.

Attività 37

It is now matter of establishing the nature of the electrical charges involved in the process. Students are asked to discuss different possible candidates. It should be borne in mind that students are already familiar with the concept of ion, both from the physics course and from their knowledge of the periodic table, electronic configurations, first ionization energies and electron affinities. So they already know that a neutral atom can lose or pick up electrons, thus turning into a charged species.

Object of the proposed activity	Learning objectives
The condition in which NaCl conducts electricity is identified and the possible agents responsible for this property are examined.	To hypothesize the presence of ions in molten NaCl or in NaCl solutions

We verified that sodium chloride does not conduct electricity when it is in the solid state, while it is a good conductor in the liquid (molten) state or in aqueous solution. We have also ascertained that electrical conduction implies the presence of mobile charges.

1. Consider solid state NaCl. In your opinion, does it contain charged particles that can freely move in space?
 - Yes, it does
 - No, it does not
 - I cannot answer
2. If you think that solid NaCl contains charged particles that can freely move in space, which particles are these?
 - electrons
 - ions
 - protons

Justify your answer

3. Consider NaCl dissolved in water. In your opinion, which mobile charged particles are present in the solution?
 - electrons
 - ions
 - protons

Justify your answer

Students' answers are discussed under the teacher's supervision. Aim of the discussion is to highlight that solid sodium chloride has no freely moving charges, whereas these can be found in NaCl solutions. Some students may argue that electrons are endlessly moving charges: hence, they might be responsible for substance conductivity. The teacher may then highlight the logical inconsistency of this hypothesis as:

- i) electrons move in the limited space that surrounds the nucleus, as they are constrained by nuclear charge;
- ii) should electrons be responsible for NaCl conductivity, this property should be observed in the solid state, which is not the case;
- iii) should electrons be responsible for the conductivity of substances, this property should be observed in the all substances mentioned in WS 35 and 36, which is not the case.

So the electronic hypothesis fails. Similarly, protons cannot be responsible for electrical conductivity as they are 'constrained' within the nuclei of Cl and Na atoms.

The ionic hypothesis, on the other hand, seems plausible and needs to be verified.

Activity 38

Activity 38 has a dual purpose:

- i) to criticize the covalent bond model (which is the only chemical bonding model known by students so far).
- ii) to show that Sodium and Chlorine ionization leads to the achievement of full shells condition similar to Noble gases configuration, that is a stability condition.

Modelling ion formation required shifting to the nuclear-electronic representations of atoms through the electron shell model.

Object of the proposed activity	Learning objectives
Students are asked to verify the applicability of the covalent bonding model to NaCl.	To highlight the inadequacy of the covalent bonding model to the description of ionic substances. To made the covalent bonding model evolve in order to include ionic substances.

Consider the following data:

	Sodium	Chlorine
Electronegativity	0,91	3,10
Number of electrons in the outermost shell	1	7

1. Sodium chloride contains sodium and chlorine atoms held together by chemical bonds. Represent the isolated atoms of Sodium and Chlorine (i.e. atoms before the formation of the NaCl substance) by using the electron shells atomic model.

Sodium atom

Chlorine atom

2. How many electrons does sodium have in its outermost electron shell? How many chlorine does it have?

Sodium

Chlorine

3. How could sodium and chlorine reach the electronic configurations of noble gases (which we know to be particularly stable)?

Sodium

.....

Chlorine

.....

4. After looking at the electronegativity data of the two elements, based on what you learnt about bonds, what type of bond would you propose for sodium chloride? Justify your answer.

5. Try to represent the Lewis structure of sodium chloride by applying the rules of Lewis model. Justify your hypothesis.

6. After the bond between Sodium and Chlorine is formed, is the outermost shell of the Sodium atom complete?

- Yes, it is;
- No, it isn't;
- I cannot answer

7. After the bond between Sodium and Chlorine is formed, is the outermost shell of the Chlorine atom complete?

- Yes, it is;
- No, it isn't;
- I cannot answer

8. Does this bonding hypothesis justify the electrical conductivity of molten NaCl?

- Yes, it does;
- No, it doesn't;
- I cannot answer

Questions 1-3 of WS 38 focus on the electronic structure of the two isolated atoms: the presence of 1 and 7 electrons (for Na and Cl respectively) in the outermost shell is highlighted. Students should realize that the achievement of noble gases configuration corresponds to the loss and the acquisition of one electron, by Na and Cl respectively. Questions 4 and 5 require students to rely on prior knowledge: they learnt that elements with different electronegativity can form polar covalent bonds. Students are then expected to apply the Lewis model.

Here two cases may occur:

- 1) Some students might realise the impossibility to comply with the rules of the Lewis model by electron sharing (which is typical covalent bonding). If the outermost electron shells must be completely filled, then electron transfer is required. Conversely, if electron sharing has to be achieved, then a stable electronic configuration won't be attained and therefore bond formation won't be justified.
- 2) Other student might overshadow electron sharing and favor energetic motivations, i.e. the attainment of stable electron configurations through interatomic electron transfer.

Questions 6 and 7 are meant to verify the hypotheses expressed in answer to question 5 and to reaffirm that whenever bonding occurs, it implies the energetic stabilization of the system, i.e. the attainment of full electronic shells)

Question 8 helps reminding that a model is not an end in itself: it is rather an interpretive tool for specific phenomena.

As usual, students' answers are discussed in the classroom under the teacher's guidance. The expected conclusion is that **the covalent bonding model does not apply to the case of NaCl**, because sharing electron pairs does not lead to the attainment of stable configuration (actually, only the Cl atom would reach it). In addition, this model cannot explain the electrical conductivity of molten NaCl or NaCl solutions. **So a new model has to be developed.**

Activity 39

Once the covalent model has been questioned, the nuclear-electronic representations of Cl and Na atoms are re-examined: students are invited to explore how they could reach a stable electron configuration. If the hypothesis of electron sharing is abandoned, it becomes possible to formulate a plausible bonding mechanism that meet the stability requirement and allows explaining the electrical conductivity of molten NaCl.

Object of the proposed activity	Learning objectives
Students re-examine the nuclear-electronic representations of Na and Cl atoms and are suggested an alternative bonding mechanism that meet the stability criterion	To make the covalent bonding model to evolve so to include ionic substances.

Look again at the electronic configurations of Sodium and Chlorine atoms.

1. How many electrons does the Chlorine atom miss as compared to its nearest noble gas?

2. Should the Chlorine atom acquire one electron, what would it become?
 - A cation
 - An anion
 - It is not possible to answer
 - I can not answer

3. How many electrons does the Sodium atom have in excess as compared to its nearest noble gas?

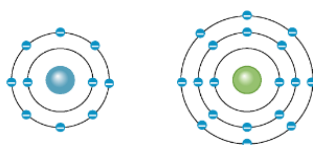
- Should the Sodium atom lose one electron, what would it become?
 - A cation
 - An anion
 - It is not possible to answer
 - I can not answer

4. Represent the Lewis structure of sodium chloride by applying the rules of Lewis model, in the hypothesis that both the chlorine and sodium atom reach stable electronic configurations after bonding.

5. Does this bonding hypothesis justify the electrical conductivity of molten NaCl?
 - Yes, it does
 - No, it does not
 - It is not possible to answer
 - I can not answer

Justify your answer.

Questions 1 and 3 focus on the stability criterion for bond formation, based on the attainment of noble gases electronic configurations. Questions 2 and 4 aims at highlighting that the application of this criterion leads to the formation of ions. This allows justifying the electric conductivity of molten NaCl (question 6). Question 5 focuses on the hypothesis of bonding mechanism. Representations of this type are expected:



Sodium

Chlorine

While discussing students' answers with the classroom, the teacher may recall the conclusions of activity 13 (based on the Lennard-Jones diagram): the main reason for the formation of an interatomic bond is the energetic stabilisation of the system. Bonding goes along an energy transfer from the system to the environment.

The classroom discussion, led by the teacher, should lead to the following shared conclusions:

- **The covalent bonding model does not justify the formation of sodium chloride.** The model need to be changed.
- Interatomic bonding is always justified by an energy transfer from the system to the environment, therefore it implies a **stabilization**. This is the only reason that justifies the formation of interatomic bonds.
- This condition occurs **when the bonded atoms attain a noble gas electronic configuration**. In the case of chlorine and sodium, this condition is met whenever the Cl atom acquires an electron and the Na atom loses an electron.
- We can plausibly assume that sodium chloride contains chloride ions and sodium ions. This justifies the electrical conductivity of sodium chloride both in aqueous solution and in the liquid state.

Activity 40

After formulating the hypothesis that NaCl contains sodium ions and chloride ions, it is necessary to analyze the implications of this statement, in order to verify the tightness of the model.

Students must be led to develop the idea that any substance, including NaCl, is electrically neutral even though it containing electrically charged particles. This implies the presence of an equal number of positive and negative charges. Furthermore, based on the electrostatics knowledge gained in WS 3 (in collaboration with the physics teacher), one can conclude that ionic bonding cannot be directional and that therefore NaCl is not a molecular substance. This activity can be carried out in collaboration with the physics teacher, given its interdisciplinary character.

Object of the proposed activity	Learning objectives
The charges that, according to the hypothesis just formulated, would be present in sodium chloride are examined and the interactions that should take place between them are analyzed.	To understand that the ionic hypothesis is plausible for sodium chloride.
	To understand that this hypothesis implies the presence of attractive and repulsive forces, in balance with each other.
	To understand that substance NaCl is electrically neutral, even though it contains positive and negative charges.
	To understand that the ionic hypothesis is incompatible with the molecular (covalent) hypothesis.

We have formulated the hypothesis that sodium chloride is formed by chloride ions (negatively charged) and sodium ions (positively charged).

1. In the light of your knowledge on the behavior of electric charges (WS 3), what kind of interaction could link these ions?
-

2. In your opinion, the substance sodium chloride is:

- Positively charged
- Negatively charged
- Neutral
- It is not possible to answer
- I can not answer

Justify your answer

3. In your opinion, sodium chloride contains:

- More cations than anions
- An equal number of anions and cations
- More anions than cations
- It is not possible to answer
- I can not answer

Justify your answer

4. Represent substance sodium chloride in the solid state at the atomic-molecular level

5. In your opinion, in sodium chloride, each sodium cation attracts one or several chloride anions?

Justify your answer

6. In your opinion, in sodium chloride, each chloride anion attracts one or several sodium cations?

Justify your answer

7. In your opinion, are there repulsive forces in sodium chloride?

- Yes, there are
- No, there aren't
- I can not answer
- It is not possible to answer

Justify your answer

8. In your opinion, in substance NaCl:

- Attractive forces between oppositely charged ions prevail over repulsive forces between ions with the same charge
- Repulsive forces between ions with the same charge prevail over attractive forces between oppositely charged ions
- Repulsive and attractive forces between ions found in NaCl balance each other
- I can't answer

Justify your answer

9. In the light of the properties of electric charges that you discussed in the previous questions, you believe that substance sodium chloride is made of:

- Molecules
- Neutral atoms
- An equal number of sodium cations and chloride anions
- Other (specify).....

Justify your answer

Question 1 recalls Coulomb's law (already discussed in WS 3) which governs the interactions between charged particles.

Questions 2 and 3 aim at underlining the neutrality of the NaCl substance, despite the presence of positive and negative charges: this condition implies a 1:1 stoichiometric ratio between cations and anions.

Question 4 aims at checking students' understanding that the ionic hypothesis involves isotropic interactions, that is bond adirectionality; therefore, the molecular hypothesis must be abandoned for NaCl.

Questions 5-8 aim to argue the implications of the ionic hypothesis and to highlight that, as is the case of covalent bonding, ionic bonding involves a balance between attractive and repulsive forces. This consideration should help highlighting the common nature of electrical interaction of both kind of bonds, despite the different bonding mechanism.

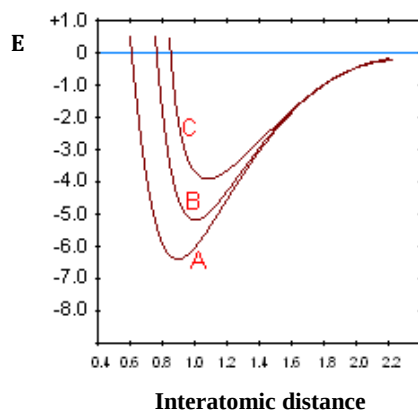
Question 9 aims at highlighting the inconsistency of the ionic hypothesis with the molecular hypothesis. It prepares the ground for the subsequent activity, focused on the isotropic character of the ionic bond.

The classroom discussion is expected to lead to the following shared conclusions:

- Sodium chloride is **electrically neutral** (like any isolated substance), and **contains an equal number of sodium cations and chloride anions**.
- Since these ions have opposite charges, they **attract each other electrically**.

- **Repulsive forces** between ions of the same sign are also found in NaCl
- Therefore, in NaCl there is a balance between attractive and repulsive forces, just like we previously discussed for the H₂ molecule.

To comment on the energetic aspects related to the formation of NaCl, the teacher can propose the following graph and resume the definition of bonding energy given after the discussion of WS 16.



The examination of the figure above and the related discussion in the classroom, led by the teacher, is expected to reach the following conclusions:

- Bonding between sodium and chlorine atoms implies the attainment of a minimum in the potential energy curve of the system.
- Bonding between sodium and chlorine atoms implies that attractive and repulsive forces are balanced.
- Among the various possible types of ion packaging in the crystal lattice, the one that maximizes the attractive forces prevails, as this maximizes the stabilization of the system (Curve A).

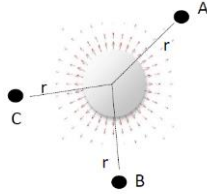
Activity 41

Activity 41 addresses some aspects related to ionic substances that are often neglected, with the result of feeding the so-called Molecular Framework.

This activity focuses on the adirectional character of ionic bonds, which derives from its very nature of Coulombic interaction between point-like electric charges: it is the key for understanding why ionic substances exhibit a reticular, non-molecular structure. In other words, ionic bonds do not involve pairs of atoms. The meaning of the NaCl notation also need to be clarified, as it designates a unit-formula and not a molecule. To this purpose, students are asked to draw the Lewis formula of an ionic compound and this notation is discussed.

Object of the proposed activity	Learning objectives
The non-directionality of charge interactions is discussed in the light of Coulomb's law.	To understand the non-directional character of ionic bonds.
The structures of a molecule and an ionic lattice are examined and the differences between them are pointed out.	To understand that ionic substances are structured in lattices and not in molecules.

Look at this image, which is meant to represent a point-like electric charge and the electric field associated with it. Three equally charged particles A, B and C are arranged at the same distance r from the electric charge.



1. In the light of your knowledge on the behavior of electric charges (WS 3), do you believe that particles A, B and C experience the effect of the electric field of the point charge:

- To an equal extent
- To a different extent
- It is not possible to answer
- I can not answer

Justify your answer.

2. In your opinion, the position of the three particles A, B and C with respect to the central charge:

- affects their interaction with the central charge
- does not affect their interaction with the central charge
- It is not possible to answer
- I can not answer

Justify your answer.

You have learned that Coulomb's law allows calculating the extent of the interaction between two charges, according to this expression:

$$F = k \cdot (|q_1 \cdot q_2|/d^2)$$

where q_1 and q_2 represent two charges and d is the distance between them.

3. In your opinion, the expression of Coulomb's law suggests:

- that the interaction between charges depends only on the entity of the interacting charges
- that the interaction between charges depends on the mutual orientation of charges
- that the interaction between charges depends only on the distance between the interacting charges
- that the interaction between charges depends on both the distance and entity of the charges, but not on their mutual orientation.
- I can't answer

Justify your answer.

We hypothesized that the NaCl substance is made up of an equal number of cations and anions, that is, oppositely charged particles. Each charged particle is associated to an electric field similar to that shown in the previous figure.

4. In your opinion, in sodium chloride:

- Each cation attracts only one anion
- Each cation repels only one cation
- Cations and anions interact with each other in all directions of space
- Each anion repels only one anion
- I can not answer

Justify your answer.

Look at this figure:

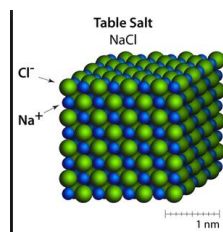
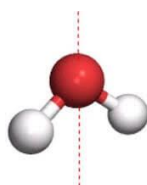


5. In your opinion, this representation of the structure of sodium chloride is:

- Correct
- Not correct
- I can not answer

Justify your answer.

Look at this figure that aims at representing the structure of a water molecule and the structure of sodium chloride:



6. You learnt that the stick that links the O and H atoms in water represents a shared electron doublet. In your opinion, why does the representation of sodium chloride not have sticks and depicts many particles instead of just a single pair?

7. In the light of what you learnt, which of the following statements is correct, in your opinion? (multiple choices are possible)

- The bond between sodium and chlorine in sodium chloride is characterized by a preferential direction, i.e. it is directional
- The bond between oxygen and hydrogen in water is characterized by a preferential direction, i.e. it is directional
- The bond between sodium and chlorine in sodium chloride is not characterized by a preferential direction, i.e. it is non-directional

Justify your answer _____

Questions 1-3 rely on the student's knowledge about Coulomb's law and the electrostatic interaction between point charges. They aim at pointing out the non-directional character of these interactions. Questions 4 and 5 require the application of these very same notions to the specific case of sodium chloride. The meaning of *sticks* is also recalled: it represents covalent bonds, i.e. a shared electron pair, and it shows the directional character of these bonds; hence, it cannot apply to NaCl. Question 6 aims at leading students to draw the consequences of previous considerations: if charge interactions are not directional, the bonds found in NaCl cannot be directional; consequently, ionic bonding cannot generate molecules. Question 7 still focuses the directional and non-directional character of covalent and ionic bonds, respectively.

As usual, students' answers are discussed in the classroom under the teacher's guidance. The following general conclusions are expected to be shared in the classroom:

- Substance NaCl consists of Na^+ cations and Cl^- anions bonded together by ionic bonds.
- These bonds are electrical interactions
- From the nuclear-electronic viewpoint, ionic bonds form when Chlorine, a very electronegative element, picks up an electron from Sodium, an electropositive element
- From a nuclear-electronic viewpoint, ionic bonding involves only electrons from the outermost electron shell. The electrons of the core are not involved in bonding.
- Electron transfer between Sodium and Chlorine atoms, which results in bonding, implies the stabilization of the system, as these atoms attain a noble gas electronic configuration.
- Contrary to covalent bonding, that generates molecules, ionic bonding generates lattices, wherein charge attractions and repulsions are balanced.
- This occurs because charge interactions are not directional.
- The NaCl symbol does not designate a molecule, but a unit-formula: it specifies the elements found in the ionic compound and the stoichiometric ratio between Na^+ and Cl^- ions in the ionic lattice.
- The energy that is released in the formation of the ionic lattice is called reticular energy.
- The stronger the ionic bond, the greater its reticular energy.

Activity 42

The previous remarks refer to NaCl: they need to be **generalized** to all ionic substances.

The teacher asks the class to consider a few ionic substances, e.g. CaCl_2 , Na_2O , MgO and to determine $\Delta_{\text{electronegativity}}$ between their elements, to build their Lewis structures and to check that bonding leads to noble gases configurations.

WS 42

Build the Lewis structure of calcium chloride (CaCl_2) after verifying the electronegativity difference between Calcium and Chlorine. What is the charge of the chloride ion? What is the charge of the calcium ion? Write their electronic configurations.

Build the Lewis structure of sodium oxide (Na_2O) after verifying the electronegativity difference existing between sodium and oxygen. What is the charge of the sodium ion? What is the charge of the oxide ion? Write their electronic configurations.

Build the Lewis structure of magnesium oxide (MgO) after verifying the electronegativity difference between magnesium and oxygen. What is the charge of the magnesium ion? What is the charge of the oxide ion? Write their electronic configurations.

Students' answers are shared in the classroom. The discussion is expected to highlight that: i) when two elements show very different electronegativity values, electron transfer is a more likely event than electron sharing; ii) a look at the periodic table suggests that ionic substances are preferentially formed by alkaline or alkaline-earth metals and non-metals; iii) formulas of ionic compounds are only meant to indicate the element composition of ionic compounds and the stoichiometric ratio between cations and anions; by no means they designate molecules.

Similar exercises as WS 42 are assigned to students as homework. Finally, the remarks previously referred to NaCl can now be generalised to all ionic substances:

- Ionic substances consists of cations and anions bonded together by ionic bonds.
- These bonds are electrical interactions
- From the nuclear-electronic viewpoint, ionic bonds form when a very electronegative element picks up electrons from an electropositive element
- From a nuclear-electronic viewpoint, ionic bonding involves only electrons from the outermost electron shell. The electrons of the core are not involved in bonding.
- Electron transfer between electronegative and electropositive atoms, which results in ionic bonding, implies the stabilization of the system, as these atoms attain noble gas electronic configurations.
- Contrary to covalent bonding, that generates molecules, ionic bonding generates lattices, wherein charge attractions and repulsions are balanced.
- This occurs because charge interactions are not directional.
- The generic formula AB of an ionic substance does not designate a molecule, but a unit-formula: it specifies the elements found in the ionic compound and the stoichiometric ratio between cations and anions in the ionic lattice.
- The energy that is released in the formation of the ionic lattice is called reticular energy.
- The stronger the ionic bond, the greater its reticular energy.

Activity 43

The last two activities of this segment the teaching sequence get back to consider some physical properties of ionic compounds, namely their high water solubility.

In order to explain this property, students are asked to to represent the solubilization process of sucrose and sodium chloride at the particle level and to specify the type of interactions found in these systems. In the case of sucrose, hydrogen bonds should be mentioned. In the case of NaCl, a new type of bonding interaction has to be introduced: ion-dipole bonds.

Object of the proposed activity	Learning objectives
Students are asked to justify the solubility of NaCl and sucrose in water and to represent the solubilization process at the particle level.	To understand that solubility depends on the type of interaction(s) that establishes between solute and solvent. To formalize a new type of bonding interaction: ion-dipole bonds.

Both sucrose and sodium chloride substances are water soluble.

1. In the light of what you learnt about bonds, try to represent the dissolution of sucrose in water by means of a particle representation at the atomic-molecular level.
2. In the light of what you learnt about bonds, try to represent the dissolution of sodium chloride in water by means of a particle representation at the atomic-molecular level.
3. Sucrose contains polar covalent bonds and its molecules are dipoles. What kind of interaction do you think they establishes with water?
 - Covalent bonds
 - Instant dipole-instant dipole bonds
 - Dipole-dipole bonds
 - Hydrogen bonds
 - Other (specify)

Justify your answer_____

4. If sucrose dissolves spontaneously in water, do you think that the bonds between sucrose and water molecules are:
 - Stronger than bonds between sucrose molecules alone
 - Weaker than bonds between sucrose molecules alone
 - It is not possible to answer
 - I can not answer

Justify your answer_____

5. Sodium chloride contains ionic bonds: therefore, it is made of ions. What kind of interaction do you think it establishes with water?
 - Covalent bonds
 - Instant dipole-instant dipole bonds
 - Dipole-dipole bonds
 - Hydrogen bonds
 - Other (specify)

Justify your answer_____

6. If sodium chloride dissolves spontaneously in water, do you think that the bonds between chloride and sodium ions and water molecules are:
 - Stronger than bonds between sodium and chloride ions
 - Weaker than bonds between sodium and chloride ions
 - It is not possible to answer
 - I can not answer

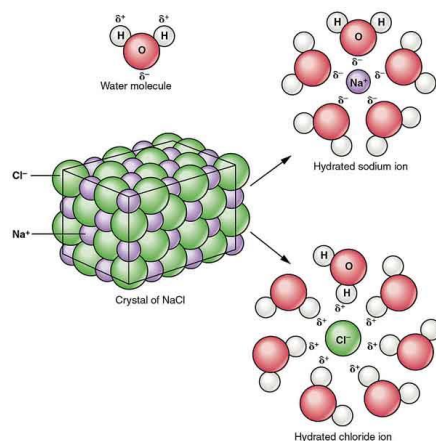
Justify your answer_____

The first questions of this WS should quickly lead students to recognize that sucrose and water are both polar substances and therefore their molecules behave like permanent dipoles. Then, the interaction between sucrose and water is dipolar.

Question 4 deals with the energetic aspects of the process in a purely qualitative fashion. The teacher reminds the energetic principle that justifies interatomic bonding: if a process occurs spontaneously, the resulting system must have a lower energy content than the starting one.

Questions 2 and 5 propose the case of sodium chloride in water. The discussion in the classroom is expected to lead students to the conclusion that the water dipole can interact with ions, i.e. charged particles. The teacher informs students that these bonds are known as **ion-dipole** bonds: once again, these are electrical interactions. Question 6 brings back the focus on the energetic aspects of NaCl dissolution in water, on a purely qualitatively basis.

To support students' understanding, the teacher may show students images like this:



Activity 44

The last activity of this segment of the teaching sequence leads students to apply their knowledge of the ionic bonding model to justify those macroscopic properties of ionic substances listed in Table 4.1 that have not yet been examined (namely, their physical state at room temperature and pressure, their high melting temperatures and their fragility). As usual, students are invited to seek a microscopic interpretation for these properties.

Object of the proposed activity	Learning objectives
Some macroscopic properties of the ionic substances are interpreted through the ionic bonding model.	To check the plausibility and effectiveness of the ionic bonding model in accounting for the properties of ionic compounds. To check students ability to apply their knowledge to solve problem-situations

Look at Table 4.1 and answer the following questions:

1. In the light of what you learnt about ionic compounds, why are they solid at room T and P?

2. In the light of what you learnt about ionic compounds, why have they high melting and boiling temperatures?

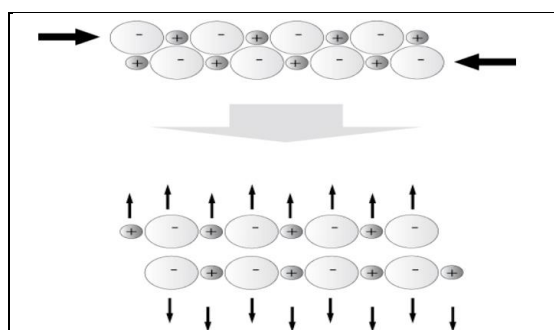
3. In the light of what you learnt about ionic compounds, why are they fragile, i.e. they shatter easily?

The discussion of question 1 and question 2 is expected to lead students recognize that the physical state of a substance at a given temperature is related to the extent of bonding interactions between the constituent particles of the substance. Ionic interactions typical of crystal lattices are highly energetic. This conclusion is supported by the experimental data shown by the teacher:

	Li⁺	Na⁺	K⁺	Rb⁺	Cs⁺
F⁻	1004	900	795	761	724
Cl⁻	808	770	703	665	623
Br⁻	766	736	661	640	602
I⁻	715	674	623	602	569

Table 4.2 Lattice energies of alkaline halides (kJ/mol)

The discussion of question 3 might raise more problems, but some students might be able to propose a suitable explanation on their own. If not, the teacher suggests an explanation by using figures like the one below, in order to highlight the combination of electrical and mechanical factors that determine the fragility of ionic crystals.



Activity 45

In conclusion of this segment of the teaching sequence, and before tackling the metallic bonding model, students were asked to accomplish the classification of substances of Table 4.1. The sets of substances designated with A, B, C, etc. can now be named after a more informative nomenclature. Students are expected to easily recognize covalent and ionic substances, based on their present knowledge on bonding model¹⁵. Metallic substances will be recognized as such on a phenomenological basis. The obvious difference between these substances and the previous ones stimulates the classroom to open a new exploratory chapter, devoted to modeling a new type of bond.

4.6 Metallic bonding model

Literature data report that students experience relevant learning difficulties face to the metallic bonding model. This is often proposed in inconsistent and hyper-simplified ways: metallic substances are often described as systems made up of positive ions floating into a sea of valence electrons. According to several authors (Cheng and Oon, 2016; Bergqvist, 2016), misconceptions on this bonding model may be reduced by making explicit the electrostatic nature of the interaction between metal atoms, as it involves positively charged atomic cores and valence electrons of metal atoms. The representation of metal-metal bonds is problematic, as well: Coll and Taylor (2001) criticize the use of *stick-and-ball* models to represent metal lattices (see figure 4.7), as these foster the misconception according to which metal substances contain molecules or covalent bonds. In fact, students associate (correctly!) each *stick* to a covalent bond, according to the previously learnt convention.

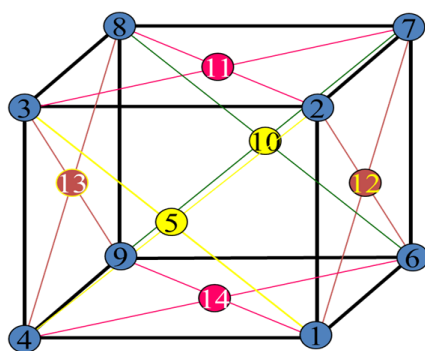


Figure 4.7 Representation of the face-centered cubic cell typical of many metals

Acar and Tarhan (2007) argue that students mix up metal and ionic bonds, because metal and ionic substances share some physical properties, namely high melting points and electrical conductivity. Confusion with covalent bonds is due, instead, to electron sharing between metal atoms. Finally, a strong belief that metal bonds are weak as metals are malleable is reported.

An opposite misconception is reported by Taber (2001): many students believe that no chemical bonds are found in metals, as the interaction that holds metal atoms together is not perceived as a chemical bond.

This teaching sequence addresses metallic bonding through the "*sea of electrons*" model, paying attention not to feed the above-discussed misconceptions. The advantage of this model lies in its being based on concepts that are familiar to students (e.g. electrostatic interaction, atomic core and bonding electrons). A more sophisticated model is proposed by many textbooks (for example Atkins, Overton, Rourke, Weller, Armstrong, *Inorganic Chemistry*, 2006, OUP Oxford): metallic substances can be described as macrostructures, whose

¹⁵ Covalent lattices, which have not been covered, will be resumed at the end of the sequence. This will allow classifying quartz in a more consistent fashion.

molecular orbitals originate from the superposition of single atomic orbitals. We believe quantum descriptions to be beyond the grasp of high school students.

The activities of this section engage students in modelling metallic bonds. At first, some macroscopic properties of metallic substances are examined (electrical conductivity, malleability, ductility, physical state at room temperature and pressure, melting points, density). Then students are stimulated to seek for their interpretation at the microscopic level. Once again, the applicability of the previously learnt bonding models is checked: these models prove unfit to provide consistent interpretations to the properties of metallic substances. Hence, a new interpretive model has to be built. The new model is therefore built as a 'critique' of previously learnt model.

Students already know that electrical conductivity of substances implies the presence of mobile charges: so, it is matter of identifying the nature of charges responsible for electrical conductivity in metals. The fact that - unlike ionic compounds - metals conduct electricity in the solid state allows discarding the hypothesis that conductivity is due to ions. The mobility of electrons has been highlighted in several previous activities. However, in order for electrons to be responsible for electric conductivity, one has to assume that electrons are not localised close to a specific atomic core (as in the ionic and covalent bonding models). They need to be able to freely move amongst several atomic cores. It is then matter of assessing the hypothesis that bonding electrons can be shared among several atomic cores, with all its implications. A second aspect that must be kept in mind is the fact that metallic substances are made of atoms of the same type: hence, $\Delta_{\text{electronegativity}} = 0$. This supports the hypothesis that outer shell electrons are shared between metal atoms, as in pure covalent bonds. But, unlike simple covalent substances, metals are conductors.

Based on these considerations, the hypothesis of a lattice is formulated, whose (positively charged) nodes are the cores of metal atoms and outer shell electrons may freely move between them. Outer shell electron neither belong to a specific core nor are shared between pairs of atoms: they are rather shared amongst all the atomic cores in the structure, thus generating a metal lattice (see Figure 4.8).

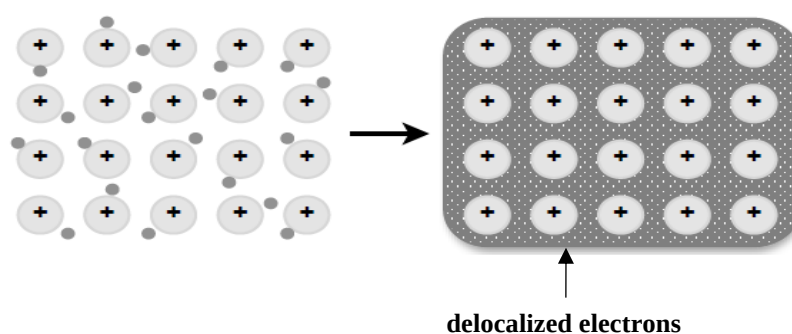


Figure 4.8 Representation of metal cores and related delocalized electrons

As in previous bonding models, the metal lattice is characterised by the balance of repulsive and attractive forces. Delocalized electrons shield the atomic cores and help minimizing the repulsions between positively charged atomic cores. As a result, each core tends to be surrounded by the largest possible number of other cores, compatibly with the geometric limitations imposed by the system: hence, the very dense packing that explains the usually high density of metal substances. Unlike in the covalent bonding model, where the number of bonds exhibited by each atom is limited by the number of electron pairs that can be shared to ensure the attainment of noble gases configurations, here geometrical factors are at play. In addition, this bonding model implies that metal bonds are not directional, for the same reasons already discussed for ionic substances.

In conclusion, this model posits the non-directionality of metal bonds, and it justifies electrical conductivity in the solid state (which is peculiar of metals, unlike covalent and ionic substances), the generally high melting temperatures and densities of metals.

The last step of the sequence is a summary, aimed at verifying the effectiveness of this bonding model in the interpretation of metals physical properties.

Activity 46

The first activity of this segment of our teaching sequence focuses on the peculiar physical properties of metallic substances as compared to ionic and covalent substances.

Emphasis is put on electrical conductivity in the solid state, as students need to realize that it cannot be explained according to the same criteria applied to ionic substances.

Object of the proposed activity	Learning objectives
Students are asked to summarize the typical properties of ionic, covalent and metallic substances. They are invited to think about the possible microscopic explanation of electrical conductivity in solid state metals as compared ionic substances.	To understand that electrical conductivity in solid state metals cannot be mediated by ions (as in ionic substances) To hypothesize the involvement of electrons in this phenomenon.

Resume the data collected in activity 4.1.

Substances exhibit various macroscopic features, such as: fragility, electrical conductivity (in different physical states), solubility in water, malleability and ductility, high melting temperatures, high density.

1. Which properties are specific to metallic substances?

2. Which solid state substances are conductors of electricity?

- Ionic
- Covalent
- Metallic
- I can not answer

3. Which substances conduct electricity when they are dissolved in water?

- Ionic
- Covalent
- Metallic
- I can not answer

You learnt that electrical conduction is mediated by freely-moving charged particles.

4. Consider metallic copper. In your opinion, which mobile charged particles are present in the substance at the solid state?

- Cu^{2+} cations
- Protons found in the nuclei of Cu atoms
- The positively charged kernels of Cu atoms
- Electrons belonging to Cu atoms

Justify your answer

5. Consider the ionic substance NaCl dissolved in water. In your opinion, which mobile charged particles are present in the solution?

- free electrons
- Protons found in the nuclei of Na and Cl atoms
- the positively charged kernels of Na and Cl atoms
- the Na^+ and Cl^- ions

Justify your answer

The discussion in the classroom, led by the teacher, is expected to highlight that solid state metals, unlike ionic substances, may conduct electricity. In fact, ionic substances act as electrical conductors only in solution or in the molten state. This property of ionic substances has been explained by the presence of freely moving ions. In the solid state, ions are immobilized so they cannot mediate the conduction of electricity.

This is true for solid-state metals as well: yet, electric conduction is possible. The classroom reaches the conclusion that **the only plausible candidates for electric conduction in solid state metals are electrons, as they are mobile charges**. The mechanism of conduction needs to be explored.

Activity 47

This activity considers the bonding models developed so far and verifies their ineffectiveness in justifying the conductivity of metals in the solid state. The questions of WS 47 also aim at highlighting that the application of covalent or ionic models to metallic substances does not meet the stability condition, i.e. these models do not lead to the attainment of noble gases configurations. A new bonding model is then required.

Object of the proposed activity	Learning objectives
The ineffectiveness of the ionic and covalent bonding models to justify the stability and the properties of metallic substances is verified.	To understand that the ionic and covalent bonding models do not meet the previously established stability requirements for bond formation in metal substances.

Represent the Sodium atom at the nuclear-electronic level, by using the electron shells atomic model

Sodium atom

1. In your opinion, in the metallic substance Sodium, are there bonds between Sodium atoms?

- Yes, there are;
- No, there are not;
- I can not answer;
- it is not possible to answer

Justify your answer

You learnt two bonding models, the covalent bonding model and the ionic bonding model.

2. Do you think two Sodium atoms in metallic Sodium can bind together by sharing pairs of electrons from their outermost shell, as it happens in covalent compounds like O₂?

- Yes, they do;
- No, they don't;
- I can not answer;
- it is not possible to answer

Justify your answer

You learnt that covalent bonds are formed whenever two neighboring atoms manage to attain a noble gas configuration by sharing electron pairs.

3. In your opinion, should two Sodium atoms be bound by covalent bonds, would they attain a noble gas configuration?

- Yes, they would;
- No, they wouldn't;
- I can not answer;
- it is not possible to answer

Justify your answer

4. You learnt that covalent bonding occurs when electron pairs are shared by two contiguous atoms; therefore they are localised around two atomic kernels. Should this happen in metallic substances, could we explain why metals conduct electricity in the solid state
- Yes, we could;
 - No, we couldn't;
 - I can not answer;
 - it is not possible to answer

Justify your answer

5. In your opinion, can Sodium atoms bind to each other by donating or acquiring one or more outermost electrons, as it happens in ionic compounds such as NaCl?
- Yes they can;
 - No, they cannot;
 - I can not answer;
 - it is not possible to answer

Justify your answer

6. You learnt that ionic bonding implies transferring / acquiring one or more electrons between two neighboring atoms so that these atoms attain noble gas configuration. Should two sodium atoms be linked by ionic bond, would they attain noble gas configurations?
- Yes, they would;
 - No, they wouldn't;
 - I can not answer;
 - it is not possible to answer

Justify your answer

7. You learnt that ionic bonding implies that electrons are localised around the nuclei of the bonded atoms. Should this happen in metallic substances, could we explain why metals conduct electricity in the solid state?
- Yes, we could;
 - No, we couldn't;
 - I can not answer;
 - it is not possible to answer

Justify your answer

The classroom discussion, led by the teacher, is expected to lead to the following shared conclusions:

- In the metallic substance Sodium, **Na atoms are bonded together**, otherwise the substance would not subsist.
- Neither the covalent nor the ionic bond model are able to justify the electrical conductivity of Sodium in the solid state, as these models predict that the electrons are localised next to specific atomic cores.

- Furthermore, neither of these bonding modes would lead sodium atoms to attain a noble gas configuration, which previous bonding models identified as the necessary condition for bonding.
- **It is therefore necessary to develop a new model.**

Activity 48

This activity aims at identifying the features useful for the construction of a bonding model suitable for interpreting the behavior of metallic substances. The students developed the idea conductivity of metals in the solid state can only be explained by hypothesizing the presence of freely moving electrons. It is now matter of identifying which electrons are likely to free themselves from their original atoms and what forces keeps metal atoms bonded together.

Students have already worked out the concept of atomic core and outer shell electrons. They also learnt that **only the latter** are involved in bonding, as core electrons are strongly attracted by nuclear charge. It is therefore reasonable to hypothesize that electrical conduction in metals is related to outer shell electrons.

Object of the proposed activity	Learning objectives
Students are engaged in the construction of a new bonding model that can justify the electrical conductivity in the solid state, which is a peculiar metals' feature.	To build a plausible bonding model for metals.

Questions 1 and 2 in WS48 aim at making students think about the stabilization associated with the loss of electrons by metal atoms: this phenomenon was previously discussed in relation to ionic bonding. However, that model does not fit to metallic substances because these are made up of atoms of the same element. Question 3 aims at reminding that the removal of one or more electrons from an atom's outer shell results in the formation of a positively charged core, capable of interacting with other charges.

Question 4 suggests a hypothesis that has not yet been explored: the possibility that bonding electrons are released from their cores and move freely amongst positively charged atomic cores. Question 5 focuses on the representation of metal structure made by a student. Students are asked to criticize it and to propose alternative solutions.

Take a look at the electron shells atomic model of the Na atom that you drew in WS 47. You learnt that, within an atom, we distinguish between the kernel (nucleus + electrons of the inner shells) and electrons of the outermost shell. By studying the covalent and ionic bonding models, you learnt that only electrons of the outermost atomic shell participate in bonding.

Consider simple substance Sodium, which contains only Sodium atoms bonded together.

1. Could we move an electron away from each Na atom, which condition would be attained:
 - more stable than the isolated Sodium atom;
 - less stable than the isolated Sodium atom;
 - it is not possible to answer;
 - I can not answer.

Justify your answer

2. In the ionic bonding model, metal atoms donate one or more electrons to non-metal atoms to get a noble gas configuration. Consider that simple substance Sodium contains only Sodium atoms. Is it likely that one Sodium atom donates one electron to another Sodium atom?
 - Yes, it is;
 - No, it is not;
 - it is not possible to answer;
 - I can not answer.

Justify your answer

3. Should an electron be removed from each Na atom present inside the metallic substance Sodium, what would remain of that atom?
 - its positively charged nucleus;
 - its positively charged kernel;
 - it is not possible to answer;
 - I can not answer.

Justify your answer

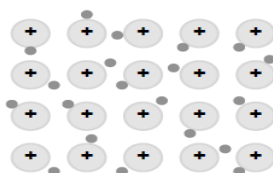
4. Should an electron be untied from each Na atom present inside the metallic substance Sodium, so that it can move between all sodium kernels, would this justify the electrical conductivity of metallic substances in the solid state?
 - Yes, it would;
 - No, it wouldn't;
 - no it is not possible to answer;
 - I can not answer.

Justify your answer

We are seeking a bonding model able to justify the following evidence:

- a metallic substance conducts electricity in the solid state
- a metallic substance is made up of atoms of the same type, which are bonded together
- the formation of the bonds is always justified by the system's stabilization

5. When asked to represent the metallic bonding model for simple substance sodium, a student proposed the following drawing. He explained that *"in the drawing I made, each positive center represents a kernel and the smallest circle the electron"*.



In your opinion, is this representation consistent with the above-listed properties of metallic substances?

- Yes, it is;
- No, it is not;
- it is not possible to answer;
- I can not answer.

Justify your answer

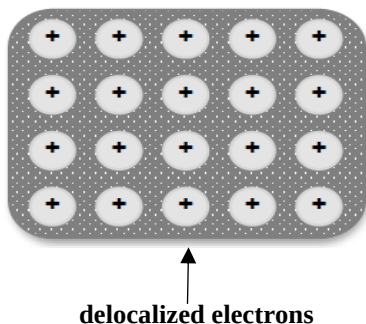
6. If you disagree with the above representation, make your own representation of metallic bonds in Sodium.

Representation of metallic bonds in Sodium.

After letting students work in small groups, the classroom is engaged in the discussion of the outcomes of groups' activity. Under the teacher guidance, inconsistencies between the representation proposed in question 5 and the properties of metallic substances are expected to come out:

- if metal atoms are bonded, outer shell electrons must participate in bonding: this implies that they won't belong any longer to their original atoms. Sharing should occur, at least to some extent;
- as all atomic cores are equal, there is no reason why electron should be shared between atoms' pairs: they should rather be equally shared among equal atomic cores. This implies that outer shells electrons are no longer constrained by single atoms, they become of moving amid atomic cores;
- the image in question 5 is inconsistent, as it suggests the idea that each electron keeps bound to its own core.

After commenting on the representations proposed by students, the teacher shares the following representation of metallic bonding with the classroom: here **outer shell electrons are no longer bound to their original cores, but are free to move among all cores.**



The teacher remarks that the logical implication of this model is that **metallic substances are organised in lattices, whose nodes are occupied by atomic cores. Outer shell electrons are equally shared by all atomic core and they move amid the cores: this explains why metallic substances in the solid state behave as electrical conductors.**

Since this image has the limit of being static, the teacher may propose students to watch part of a video (minutes 1.26 to 2.36) available at URL: <https://www.youtube.com/watch?v=S08qdOTd0w0>. This video helps imagining electron delocalization between the cores of a metal lattice. The teacher points out the purely demonstrative character of this video, that disregards the fact that atomic cores of the lattice are not steady, as they oscillate around their equilibrium positions.

Activity 49

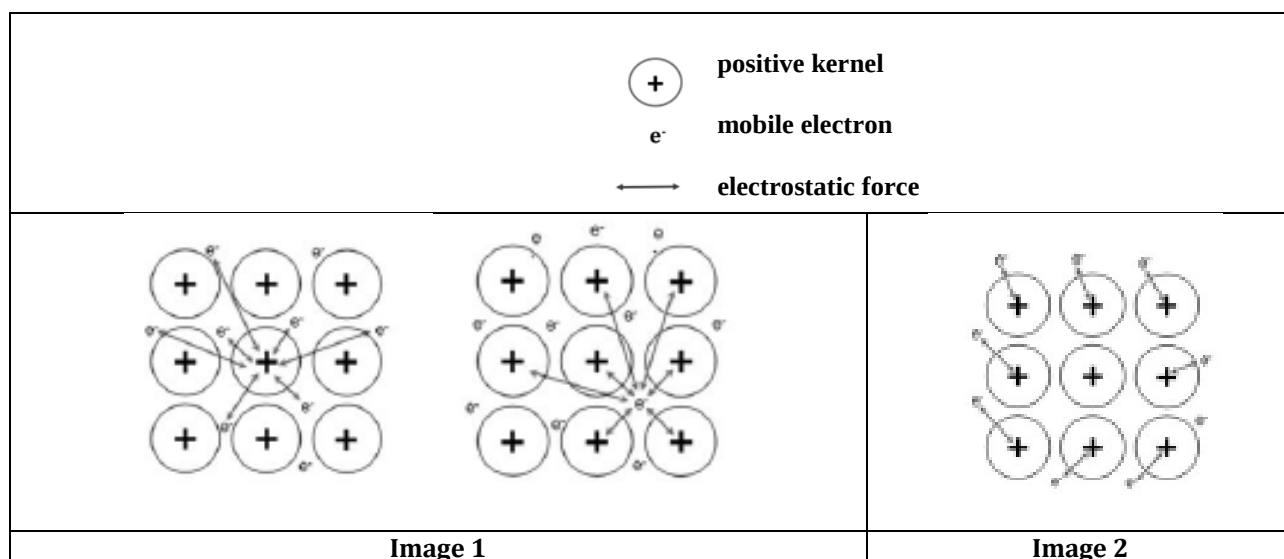
It remains to clarify which forces are at play within the metal lattice. If the lattice is made up of positively charged cores, electrical repulsion is expected to occur between them, as well as between the delocalized electrons. On the other hand, negatively charged electrons are expected to be attracted by the positively charged atomic cores. Only the balance of attractive and repulsive forces allows metal atoms to remain cohesive.

Object of the proposed activity	Learning objectives
Some features of the metal bonding model are discussed with students.	To understand that electrical interactions within the metal lattice are isotropic and metal bonds are non-directional. To strengthen the concept that metal bonds are electrical interactions: the metal lattice derives from the balance of attractive and repulsive electrical forces between the system’s constituents.

To highlight these aspects, the instrument of class discussion is used, regardless of the usual help of a worksheet.

The teacher will show the students images 1 and 2, specifying that they are symbolic representations of a metal lattice. Then he will ask the students the following question:

In the light of what we learnt on the metallic bonding model, which of these two images represents *metallic bond* most coherently, in your opinion?



After giving students time to analyse these images, the teacher leads the discussion by asking further questions, such as:

- The positively charged atomic cores of metals are represented inside the lattice: what kind of interaction do you expect to take place between them?
- Inside the metal lattice, bonding electrons are known to move freely between the atomic cores: what kind of interaction do you expect to take place between these electrons?
- What kind of interaction do you expect to take place between these electrons and the atomic cores?
- Are electrostatic interactions directional?
- In your opinion, which kind of interactions prevail within the metal lattice:
 - i) repulsive interactions
 - ii) attractive interactions
 - iii) the two types of interaction are counterbalanced

The first image aims at highlighting the isotropic character of electrostatic interactions. This means that (i) each electron interacts with all atomic cores in the lattice; (ii) each atomic core interacts with all electrons. The second image (similar to that found in WS 48B) shows these interactions as if they involved just one core and one electron.

The purpose of this discussion is threefold: **i) to emphasize that metallic bonds are not a directional; ii) to point out that metallic bonds, just like any other previously discussed type of bonds, involve electrical interactions; iii) to highlight that the metal lattice is the result of a balance between attractive and repulsive forces.**

At the end of the discussion, the teacher shares the following conclusions with the classroom:

- **Metallic bonds are electrical interactions between metal atoms that involve outermost shell electrons and positively charged cores of metal atoms.**

- According to the metal bonding model, outershell electrons are shared between all metallic cores in the lattice. As a metal is made up of atoms of a same element, bonding electrons are equally shared among metallic cores in the lattice and move freely amongst them.
- The electric interactions in the metal lattice are non directional, i.e. the metallic bond is not directional. Metallic substances are reticular substances: they are not made of molecules.
- Attractive and repulsive forces are balanced within the metal lattice: this fact determines the stability of the system.
- The ability of solid-state metallic substances to conduct electricity is explained by the property of bonding electrons to move freely amongst atomic cores.

Activity 50

Once the metal bonding model described, it is advisable to get back to the macroscopic level and take into account those properties of metals that have not yet been discussed (e.g. the physical state at room T and P, melting points, density, malleability, insolubility in water) and justify them in the light of the bonding model. The density and the physical state of metals at room T and P is justified by the packaging of metal cores that results from high bonding energies; the workability of metals depends on the fact that, unlike in ionic substances, reticular planes may slide over each other without perturbing the balance between electrical forces; finally, metal insolubility in water is justified by the fact that the formation of water-metal atoms interaction is energetically disadvantaged as compared to metal bond energy.

Object of the proposed activity	Learning objectives
Students are asked to use the metal bonding model to justify the macroscopic properties of metals (insolubility in water, physical state at room T and P, melting temperatures, density and workability) listed in Table 1.	To understand that all macroscopic properties of metals may be justified by the metal bonding model.

Take a look at the data collected in Table 4.1 and answer to the following questions, in light of the metal bonding model we just developed

- In activity 43 you identified the reasons why ionic compounds are soluble in water. In your opinion, why metallic substances such as copper, iron and gold are not soluble in water?
 - Because the bonds between metal atoms are weaker than those that can be established between metal atoms and water molecules;
 - Because the bonds between metal atoms are stronger than those that can be established between metal atoms and water molecules;
 - Because the bonds that can be established between metal atoms and water molecules are very strong;
 - I can not answer

Justify your answer

- In your opinion, why metallic substances are all solid (except mercury) at room temperature and pressure?

Justify your answer

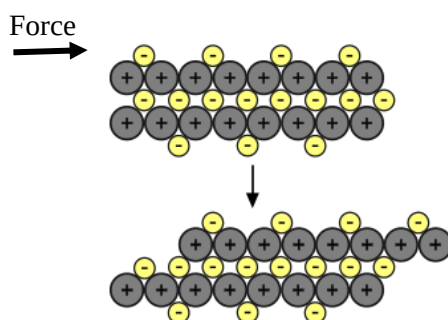
- In your opinion, why do metallic substances generally have high melting points?

Justify your answer

- In your opinion, why do metallic substances generally have high densities?

Justify your answer

- The following figure tries to explain a typical behavior of metals. In your opinion, which macroscopic property it refers to?



Justify your answer

Question 1 aims at highlighting that metals are insoluble in water because the interaction of metal atoms with water molecules is weak as compared to metal bonding energy. Therefore from the energetic

viewpoint, the solubilization of metals in water is not energetically favored; this is an opposite behavior with respect to ionic compounds and polar covalent substances.

Questions 2, 3 and 4 aims at making students think about the fact that the physical state of metals at room T and P, their melting points (which are generally high) and their generally high densities depend on the packaging of metal atoms in the crystal lattice and, ultimately, on the extent of the electrical interactions in the lattice.

Question 5 concerns malleability and ductility, two peculiar properties of metals. Students have already learnt that, in ionic lattices, the sliding of the lattice planes deeply perturbs the balance of attractive and repulsive forces: if mechanical solicitation induce repulsions to prevail, the ionic compounds disintegrate; ionic substances are fragile.

The non-fragility of metals depends on the fact that metals are made of the same kind of atoms; hence, when reticular planes slide over each other, the balance of electrical forces is not significantly perturbed. This makes the metal malleable and ductile.

At the end of the discussion in the classroom, the following conclusions are drawn:

- Metallic substances are crystalline substances, made up of atoms of the same type, which share their outershell electrons;
- Metals are insoluble substances in water because the formation of bonds between metal atoms and water molecules is energetically disadvantaged;
- The solid physical state of metals at room T and P (Hg is the only liquid metal) is justified by the high bonding energies between metal atoms;
- The fact that the densities (at 20 ° C) of metal substances are generally high is justified by the high degree of packaging of metal atoms within the metal lattice;
- The workability of metals, that is their peculiar malleability and ductility, is justified by the fact that the sliding of the reticular planes does not perturb the balance between attractive and repulsive forces within the metal lattice.

Activity 51

Now that all bonding models have been discussed, a further case remains to be taken into account: quartz, and more generally, reticular covalent solids have not yet been mentioned.

Elements, such as carbon and silicon, which have four electrons in the outermost electron shell, are capable of forming four covalent bonds and can give rise to macrostructures. These are extended structures made of very many atoms of non-metallic elements, each one bonded to the adjacent atoms through covalent bonds: therefore, these lattice structure are made of directional, bonds. Bond directionality distinguishes this type of lattices from ionic and metallic ones.

The packaging of the lattice components is determined by the number of electronic doublets that can be shared by adjacent atoms, in order to reach noble gas configurations. These structures are typical of diamond, silicon dioxide, silicon carbide (carborundum), etc.

After resuming table 4.1, students are invited to consider the substances in group C (that were previously classified as covalent). Based on the chemico-physical properties listed in the table, this group is, in fact, quite heterogeneous. The teacher underlines that quartz has peculiar characteristics as compared to the other substances in group C. For example, it has a significantly higher melting temperature, closer to metallic substances'. However, quartz is an insulator and it is insoluble in water.

Students are then invited to verify if the covalent bonding model works for quartz. The goal is to show that quartz can be effectively described according to this model, albeit its physical properties suggest its structure to be covalent and reticular (i.e. not molecular, as expected).

Object of the proposed activity	Learning objectives
Students are invited to compare the properties of quartz with those of molecular substances, of ionic and metallic substances listed in table 4.1	To apply the covalent bonding model to quartz and get covalent lattices. To justify the high melting temperature of quartz, its electrical non-conductivity and its insolubility in water at a microscopic level.

1. Quartz is a substance made of Silicon and Oxygen, according to the following formula SiO_2 . Take a look at the data of activity 1 and concentrate on the substances in group C. Compare the melting temperatures of sucrose, diiodine, sulfur and quartz. In the light of what you learnt, associate each substance in group C with the type of bond that you judge correct.

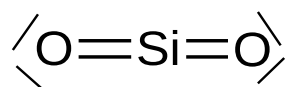
- Dipole-dipole bonds
- Covalent bonds
- Ionic bonds
- Metallic bonds
- Hydrogen bonds
- Bonds between instantaneous dipoles

Justify your answer

2. In the light of what you learnt, why is quartz insoluble in water?
- Because the bonds between silicon and oxygen atoms are weaker than those that these atoms can form with water molecules;
 - Because the bonds between silicon and oxygen atoms are stronger than those that these atoms can form with water molecules;
 - I do not know;
 - It is not possible to answer

Justify your answer

3. Look at the periodic table: silicon lacks 4 electrons to complete its outer electron shell and oxygen lacks 2. In the light of what you learnt, is the following Lewis structure plausible for quartz?

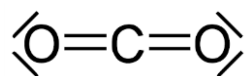


Justify your answer

4. In the light of what you learnt, which inter-molecular interactions can you predict for a substance whose molecular structure matches the one above? (multiple options are possible)
- Dipole-dipole bonds
 - Hydrogen bonds
 - Bonds between instantaneous dipoles
 - It is not possible to answer

Justify your answer

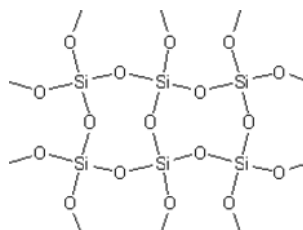
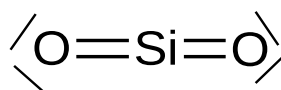
5. Carbon and Silicon belong to the same group in the periodic table. Carbon can bind two oxygen atoms to form the CO_2 molecule, which has the following Lewis structure:



Carbon dioxide is a non-polar, gaseous substance at room T and P. Quartz is a brittle and hard solid. In the light of these considerations, do you think that the quartz structure proposed in question 3 justifies its physical properties?

Justify your answer

6. Observe and compare the two Lewis structures proposed in the figure below:



In the light of what you learnt, which of the following statements is correct?

- Both of them comply with the rules of the Lewis model
- Neither of them comply with the rules of the Lewis model
- The left structure comply with them, the right one does not
- The right structure comply with them, the left one does not

Justify your answer

7. In the light of what you learnt, which of the two previous structures allow justifying the physical properties of quartz?
- The structure on the left
 - The structure on the right
 - None of them
 - I can not answer

Justify your answer

Questions 1 and 2 aim at highlighting the common covalent character of the mentioned substances, and to make the students think about the strength of inter-molecular bonds suggested by the values of melting temperatures of group C substances. Clearly, quartz exhibits an anomalous behavior as compared to the other substances of the same group.

Questions 3 and 4 focus on the Lewis structure built on the basis of Lewis model's rules. The structure is formally plausible, but leads to predictions that are inconsistent with the properties exhibited by quartz

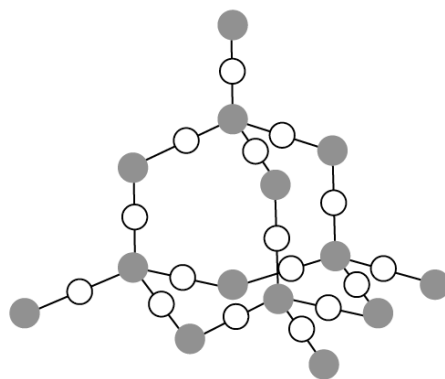
(questions 5). Questions 6 and 7 compare two structures that are plausible from the formal viewpoint, whereas only one of them is consistent with quartz properties.

The hypothesis of a covalent lattice, instead of a molecular substance allows justifying the high melting temperature and hardness of quartz, due to the fact that covalent bonds are more energetic than inter-molecular interactions. This hypothesis is also consistent with the insulator behavior of quartz.

The covalent bonding model allows modelling covalent lattices: bonding electrons are shared between atoms' pairs, so they are localized; hence, quartz is an insulator.

The teacher summarises the following conclusions:

- Quartz is characterized by covalent, directional bonds, but its structure is not molecular.
- In quartz, each Si atom binds four O atoms; each O atom binds two Si atoms. Taken together, they form a three-dimensional lattice of the type represented in the figure below.
- The high melting temperature and hardness of quartz are due its high bonding energy.
- The electrical non-conductivity of quartz is due to the fact that the electrons within the reticular structure are all localized.
- The water insolubility of quartz is due to the fact that the interactions between water and the silicon and oxygen atoms are too weak to compete with the covalent bonds found in the lattice.



Representation of the structure of silicon dioxide

The teacher remarks that a similar structure is found in other covalent such as diamond and silicon carbide (carborundum).

4.7 Conclusive summary activity

The final part of the sequence on interatomic bonding is a summary of the basic notions developed along this teaching sequence. The teacher asks students to help him listing the main features of interatomic bonds and of bonding models they dealt with:

- The bonding notion is a concept that designates the interactions between atoms
- All bonds originate from electrical interaction involving the atoms' components
- Bonds forms spontaneously whenever the resulting system is more stable than the starting system
- Despite the common electrical nature of bonds, different bonding models are needed to justify the wide range of properties observed in substances.
- Bond strengths grows approximately in the order shown in the figure 4.9:

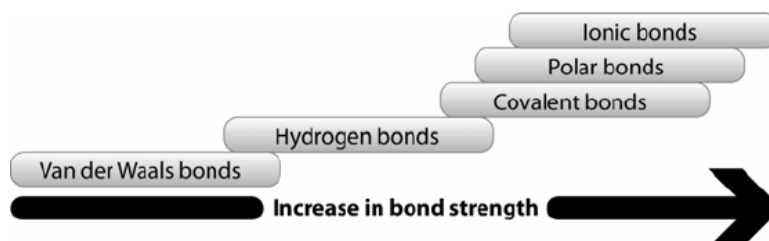


Figure 4.9 The various types of chemical bonds ordered according to an increasing energy scale (Nahum et al. 2008)

- Bonding energy corresponds to the energy required to take the entities that participates in bonding at infinite distance
- The weakest interatomic bonds are those perturbed during physical transformations of substances
- The strongest interatomic bonds are those perturbed during chemical transformations of substances
- The strongest interatomic bonds result in reticular structures (ionic, metallic and, in some cases, covalent) or in molecules (covalent)
- Interatomic bonds determine the physical properties of substances (melting and boiling temperatures, water solubility, electrical conductivity, hardness, workability, etc.) and their reactivity.

Evaluation or review activities

To consolidate or verify the achievement of learning objectives, activities such as those described below can be used.

These activities are either useful to stimulate classroom discussions (with the teacher or in small groups) or may be exploited as individual summative tests on the subject.

Activity A1

In WS A1, students are asked to complete the table drawn up at the beginning of the sequence, by associating to each class of substances the corresponding bonding model and by listing their main features. The two columns provide information referred to the macroscopic and microscopic/modeling levels, respectively, so to induce students compare the level of observation with the interpretative/predictive level.

The goal is to reinforce the idea that the bonding notion belongs to the modeling level and to consolidate students' understanding of the relationships between models and reality.

Go back to table 4.1 which lists the macroscopic properties of the different types of substances. Add a column on the right, whose heading will be “BONDING MODELS”, and fill it in, in the light of what you learnt.

(Part of the table is shown as an example)

TYPE OF SUBSTANCE	EXAMPLE	MACROSCOPIC PROPERTIES	BONDING MODELS
A IONIC SOLIDS	Sodium chloride	Solids at room T and P Non-conducting at solid state Conductor in solution Soluble in water High melting points Fragile	Electrical attraction between ions of opposite charge Reticular structure Adirectional bond
B METALLIC SOLIDS	Copper	Solids at room T and P Conductor in solid state Insoluble in water High melting points (although, quite variable from one substance to another) High density (although, quite variable from one substance to another) Not fragile	Electronic delocalization Reticular structure Adirectional bond

Activity A2

WS A2 aims at verifying students' understanding of the fact that each substance is involved in several types of bonds, whose energy scales are different.

Consider the following table and associate one or more types of chemical bond to each item, according to what you learnt on the subject:

Substances	Types of bonds
LiF	
Ag	
C	
CH ₃ OH	
N ₂	
SO ₂	

Justify your answer for each substance and specify the features of its bond's type:

LiF

Ag

C

CH₃OH

N₂

H₂O

How do you justify the fact that, at room T and P, LiF is solid, whereas N₂ is gaseous?

In your opinion, it requires more energy to bring water from the liquid to the gaseous state or to break it down into its O and H components?

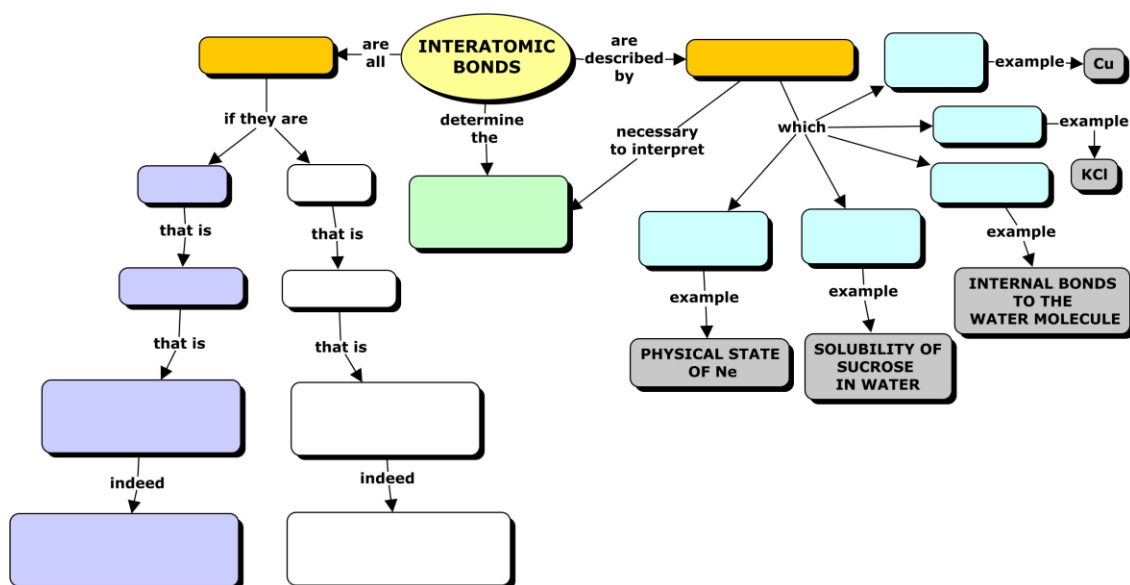
Activity A3

WS A3 requires students to complete a concept map that summarizes the main contents met during this learning pathway. Students are provided with the concepts to be used to draw up the map: the competence's assessment consist in asking them to rationally connect them. Alternatively, students may be asked to develop a map on their own.

Complete the following concept map on interatomic bonding, by using all the hints provided in the table.

Metallic bond	Weak	London Forces	Different models
Less energy is required to loosen or break the bond	Bond is less stable	In the L-J graph the potential well is deeper	Strong
Macroscopic properties of substances	In the L-J graph, the potential well is less deep	Ionic bond	Bond is more stable
Covalent bond	Electrical interactions	More energy is required to loosen or break the bond	Dipole-dipole bond

Insert each statement/word in the correct box in the map.



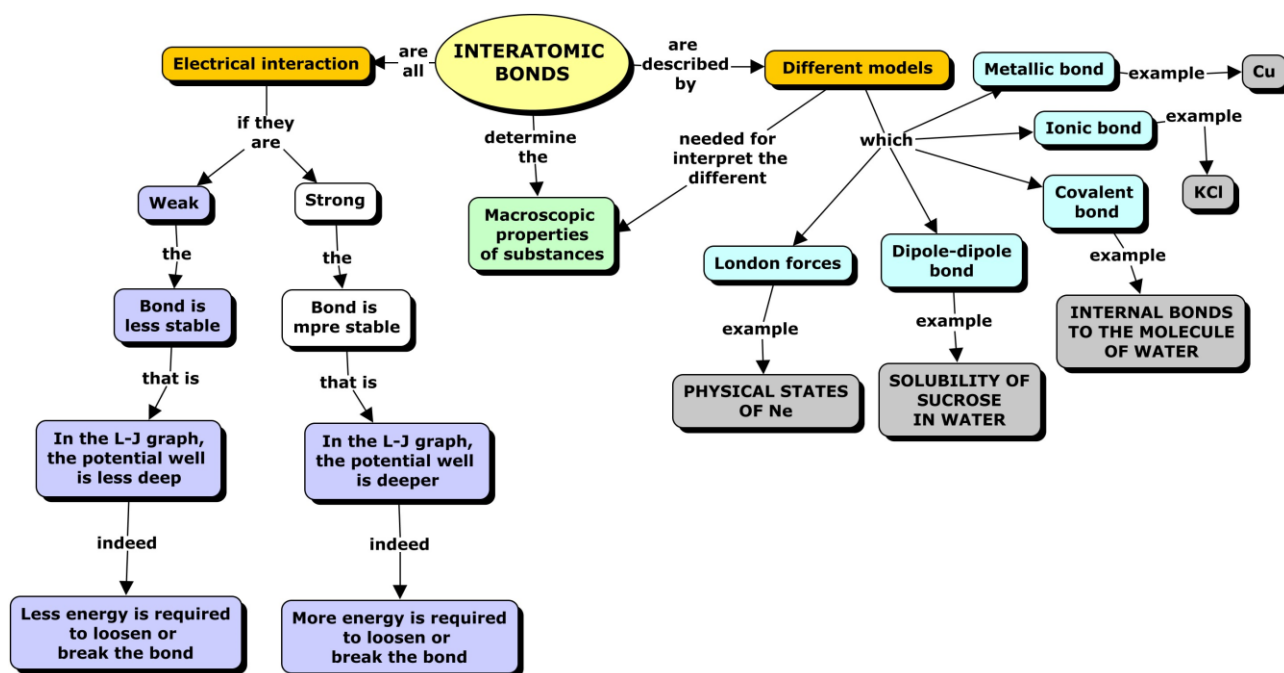
Activity A4

WS A4 requires students to associate concepts related to interatomic bonding, in order to match those that are logically related.

Draw arrows in order to match the concepts on the left to those on the right, according to what you judge appropriate.

CaCl₂		All kinds of interatomic bonds
Solid lattice		London Forces
Sharing of outermost shell electrons		Ionic bonds
Solid conductive lattice		Covalent bonds
Water-soluble solid lattice		Hydrogen bridge bonds
Electrical interactions		Ion-dipole bonds
Balance between attractive and repulsive electrical interactions		Dipole-dipole bonds
Interaction between instantaneous dipoles		Metallic bonds
Solubility of NaCl in water		
Miscibility of ethyl alcohol in water		
Interactions between permanent dipoles		
Miscibility of I₂ in hexane		
Non-directional bond		
Achievement of energetic stability		
Delocalization of bonding electrons		

The results of these activities may be discussed with the classroom or evaluated as individual tests.
The concept map that students are expected to draw in (WS A3) is as follows:



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Chapter 5

Experimentation of the didactic sequence in the classroom. Concluding remarks

5.1 Context choice and work sheets selection

The didactic sequence on the concept of chemical bond presented in the previous chapter was partially tested in the second-year class H IT ST. CMB (Istituto Tecnico Technological Sector: Chemistry, Materials, Biotechnology) of the technological high school ITIS "Q. Sella" in Biella. The class consists of 23 students. The teacher of Integrated Sciences (Chemistry) prof. Marco Ghirardi is also the co-tutor of this doctoral thesis. The weekly timetable of the Integrated Sciences (Chemistry) teaching subject includes 3 hours in the first-year class and 3 hours in the second-year class, with theoretical and laboratory lessons.

The original plan of testing the entire sequence on several classes of various schools, during the entire school year, has clashed with the limits imposed by the pandemic. Due to the health emergency, the timing and methods of experimentation have undergone considerable changes. For most of the time, the teaching activity in the school year 2020/2021 took place in remote or mixed mode (half class in the classroom, the other half online). Once established the impossibility of testing the entire sequence, at first we selected a limited number of activities (18 WS out of a total of 50 WS): we either choose those parts of the sequence that addressed the conceptual knots of bonding in an original way or those that aimed at developing students' awareness of the procedural aspects of science. The following activities were therefore chosen:

- Macroscopic properties table - aimed at stimulating the search for explanatory models at the microscopic level, starting from the observation of the diverse macroscopic properties of substances. The intent was to highlight the impossibility of resorting to a single explanatory model for such a broad spectrum of properties.
- Activity 1-8 – Aimed at building the concept of instantaneous dipole by focusing on the mobility of electrons in the atom and discussing its implications. For this purpose, the properties of monoatomic substances (noble gases) are discussed first, in order to avoid overlapping the concepts of inter- and intra-molecular bonds.
- Activities 32-34 – Aimed at consolidating the concept of dipole-dipole bond interaction, through the example of the formation of the hydrogen bridge bond, by emphasizing its peculiarities and pointing out the electrostatic nature common to all types of bonds.
- Activity 35-41 – Aimed at building the ionic bond model starting from the observation of the ineffectiveness of the covalent bond model in justifying the macroscopic properties of ionic substances. In particular, this activity insists on two aspects: i) the electrical conductivity of ionic substances in the molten state; ii) the non-directionality of ionic bonds, which results in the formation of lattices, as opposed to the directionality of covalent bonds, associated with the concept of molecule. The construction of models as a critique of previous models has the following didactic advantages: i) the plurality of bonding models is not proposed as a given fact, but arises from the explanatory needs of macroscopic reality. In fact, students are stimulated to reflect on the fact that a single type of bonding model cannot satisfy the explanatory needs deriving from the vast range of observed phenomena; ii) the reflection on the features of models, their limits of applicability and their relationship with reality.

Unfortunately, the continuous changes occurred along the year, due to the pandemic, finally made it possible to test only the first two above-listed points. The results of this activity are reported in §5.3.

5.2 Procedure for data collection

The results of the experimentation carried out in the classroom were collected through the analysis of the various WSs compiled by the students, either independently or under the teacher's assistance; we also recorded and analysed the students' feedback coming from the discussions carried out in the classroom, between the students and the teacher. An evaluation form was drawn up for each administered WS (Table 5.1):

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
Outcomes of the answers provided by students and of the shared discussion				

Table 5.1 Evaluation form of the sequence sheets

The form reports the WS number and its specific learning objective(s). The bottom row shows the outcomes of the answers of each WS, provided by individual students, and the outcomes of the shared discussion. The strengths and weaknesses of each teaching activity are underlined in the third and fourth columns. Finally, the last column reports suggestions for improving the teaching actions, to be implemented in future trials.

5.3 Results of the experimentation

This section lists the evaluation forms completed for each sheet administered to the students during the course of the experimentation of part of the didactic sequence on the concept of chemical bond.

Starting activity	Learning objectives	Strengths	Critical issues	Future improvements
Table of macroscopic properties	The goal of this activity is twofold: - To highlight the variety of behaviors and properties of the various substances and materials - To highlight the need for and to stimulate the search for explanatory models at the microscopic level.	This activity is part of the didactic approach that introduces students to the microscopic/modeling level, by highlighting the explanatory needs that emerge from the observation of macroscopic behavior of matter. In fact, the questions raised by the extensive variety of macroscopic properties urge for the elaboration of interpretative models, capable of justifying: the physical states of substances at a given T and P; the solubility/insolubility of substances in water; their electrical conductivity/non-conductivity; the fragility of materials.	Highlight the qualitative nature of the requests. The requests related to conductivity and water solubility of materials need to be reformulated in order to avoid students to look for numerical data, that are not needed for discussion purposes.	We need to explicit the fact that the numerical values of conductivity and solubility of the materials are not required, as qualitative answers are sufficient. For example, the words “Solubility in water” could be replaced with “Is it soluble in water? YES / NO / It is not possible to answer ”. In a similar way, the questions referring to electrical conductivity should be rephrased: “Does it conduct electricity at T and P environment? “Does it conduct electricity in aqueous solution?”; “Does it conduct electricity in a liquid state?”; “Is it fragile?”. In addition, we will add a note, aimed at reminding students that before answering they must make sure they know the meaning of the properties under examination.

Outcomes of the answers provided by students and of the shared discussion

Students were asked to fill Table 1 in, by focusing on the physical properties of different substances and materials. The teacher assigned the compilation of the table as a task to be carried out during the Christmas holidays (2020); the task was assigned without providing any further information, in order to bring out possible ambiguities in the assignment, to highlight the students' preconceptions and to stimulate them to ask questions or clarifications. During the winter holidays, some students contacted the teacher, through the Teams chat, and asked him the following questions: (1) *"Concerning the table, I cannot find the data of the conductivity of the various materials in water, as well as the conductivity in the liquid state. I cannot understand where I can retrieve this information, because I have searched on the internet and in the textbook, but I have not found anything about it"* (*"Per quanto riguarda la tabella non riesco a trovare i dati della conducibilità in acqua dei vari materiali e della conducibilità allo stato liquido dei vari materiali. Non riesco a capire dove devo recuperare queste informazioni, perché ho cercato su internet e sul libro ma non ho trovato niente al riguardo"*); (2) in relation to a screenshot containing the conductivity data of sodium chloride in water, the following question was asked: *"Are these the conductivity data to be reported in the table?"*, (*"Sono questi i dati di conducibilità da riportare nella tabella?"*). The teacher suggests both students to decide autonomously how to fill the table in, and anticipated that the issue would be discussed during the following lesson. This answer was justified by the need to verify how the other students would perform this task, without further instructions from the teacher.

With regard to the expected results, it should be noted that:

- The students did not have to provide the numerical solubility and conductivity values: purely qualitative answers were expected (e.g. the substance is soluble in water, the substance is an electric conductor or an insulator);
- As a result of this ambiguity, many students experienced difficulties in interpreting the numerical data obtained from the sources. Some recognized that the metallic substances listed in the table are insoluble in water, but then declared that those same substances, placed in water, were electrical conductors. Probably they were not able to recognize that a very low numerical value of water solubility means that the substance is insoluble. The poor students' understanding of the link between conductivity and solubility in water clearly emerged;
- Several students did not indicate that metals are electrical conductors in the liquid state (molten state);
- Answers concerning the fragility of substances and materials highlighted various uncertainties: several students stated that metals are fragile and/or confused the concepts of fragility and malleability/ductility.

The shared discussion highlighted the following points:

- The first aspect taken into consideration by the teacher concerned the use of the term "materials" placed at the head of the first column of the table. The teacher asks the students the following question: *"Is it possible to use a less generic term than" materials"*? The discussion starts thanks to the intervention of a student who believes it is possible *"Maybe we can use the terms element, simple substance or compound substance"* (*"Magari utilizzare i termini elemento, sostanza semplice o sostanza composta"*). During the debate following this first speech, a student reports that it would not be appropriate to use the term simple

substance or compound substance because the list includes both simple and compound substances. The teacher, in order to move the discussion forward, asks to communicate if there have been any cases in which the students have had difficulty in finding the melting temperature data. Some students report difficulties in finding quartz and PET data. The teacher asks the students how it is possible to justify this difficulty and a student explains that, during this search, he believes to have understood that there are various types of PET. The debate allows the teacher to point out the difference between mixtures and substances, both from a microscopic and macroscopic point of view. Thus, the unanimously agreed conclusion is that, since the list contains pure substances and mixtures, the use of the term “materials” is justified and vice versa the use of a “more specific” term would not be appropriate.

- The sharing of the data collected by the students and their discussion highlights that the greatest difficulties met by students involved finding the numerical conductivity and solubility values, which in fact were not required: a qualitative indication would have been sufficient. This highlighted the ambiguity of the request, which will be reformulated in the table. Furthermore, the discussion brought out what follows: a student reports that in addition to electrical conductivity there is also thermal conductivity; a student reported that he had difficulty in finding the "conductivity at the liquid state" especially for quartz; with reference to the last intervention, the teacher takes the opportunity to illustrate the various types of quartz and underlines the problematic nature of the use of the term substance with regard to this material.
- At the end of the discussion on the data in the table, the teacher underlines the variety of behaviors of the examined materials and asks students to formulate hypotheses that justify it. For example, the 'insulating' character of quartz (i.e. its inability to conduct electric current) is discussed. A student states that "*we should see how the quartz particle is made*", (*“bisognerebbe vedere come è fatta la particella del quarzo”*): therefore he refers to the microscopic level. At the start of the next lesson, the teacher asked the students: "*Do you think it is possible to group the substances in the table into homogeneous groups, based on their properties? How to justify the existence of such marked differences between one material and another?*". For lack of time, these questions were not discussed extensively. The teacher was above all concerned to share the idea that the interpretation of the macroscopic properties of the different materials requires the use of models that are located at the microscopic level (i.e. bonding models able to take these properties into account). It should be emphasized that - in the previous year - the class had already acquired the habit of connecting the macroscopic and microscopic levels of chemistry through the development of interpretative models, such as the particle model. In the light of these reflections, the teacher anticipates that the objective of the subsequent lessons will be to investigate the interatomic relationships existing in substances.

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
1	To consolidate the concept that a substance in any physical state is characterized by interacting particles. The entity of the interactions determines the physical state. The condensed states are characterized by constraints that are not present in the gaseous states.	- Discussion on the distinction between constraint and bond. - To explicit the presence of interactions (bonds) and the absence of constraints between the particles of a gaseous body, as the particles can freely move in the space available to them.	The use of the term "constraint" was problematic to students, who are not familiar with this term. Students were already aware of the relation between state of aggregation and the presence of interactions at distance (bonds) between particles, even though they did not know about their electrostatic nature, but they find difficult to distinguish between bond and constraint. In light of the experimentation, the use of the term "constraint" was not very effective and will need to be replaced.	Replacement of the term "constraint" with a more suitable terminology to convey the idea of the limitations in the mobility of particles typical of the solid state, not the gaseous one. Introduction of questions aimed at clarifying the specificity of the term "bond" intended as an interaction between particles, which is present regardless of the physical state of the substance.
Outcomes of the answers provided by students and of the shared discussion				
The particle representations of helium in the three states of aggregation, developed by the students, are consistent with what the students have learnt up to this point (and during the activities of the previous school year). Most students answer question 2 by stating that, in the solid state, helium atoms are close and ordered and this is possible thanks to the presence of constraints. A student roughly anticipates the explanation of bonding at the electron-nucleus level by citing bonding electrons. Another student reports that he cannot answer the question. The discussion in the classrooms highlights that this uncertainty is shared by other students. The teacher acknowledges the difficulty of the students to perform the assignment, and starts the discussion by asking them to explain what the term "constraint" means; he also asks to suggest synonyms. The discussion begins with the intervention of a student who states that a constraint is <i>"anything that forces something to do a certain thing or to be in a certain way; to follow a certain path"</i> (<i>"qualunque cosa che obbliga un qualche cosa a fare una determinata cosa o ad essere in un certo modo; a seguire un certo percorso"</i>); another intervention is <i>"anything that holds the atoms together, that is the synonym of bond"</i> (<i>"qualunque cosa che tiene legati gli atomi cioè il sinonimo di legame"</i>). The majority agrees with this interpretation that considers that "constraint" is synonym of bond. So, the teacher asks the students: <i>"would the term bond have</i>				

been clearer?". Everyone agrees that it would have been clearer, including students who had difficulty answering the question; a pupil says *"yes, I identified it better"* (*"sì, identificavo meglio"*).

The analysis of the students' answers to the third question of WS 1 shows that 8 students agree on the fact that constraints between helium atoms are found even in the liquid state. The justification shared by all students is that these constraints are there, but they are weaker because the particles are further away than in the solid state. Two students report instead that there are no constraints in this case, one of them does not justify the answer while the other student says that the constraints are absent because *"by taking a drop I do not break any bond"*, (*"prendendo una goccia non spezzo nessun legame"*). The discussion in the classroom has this outcome: one student says *"there are no bonds! If I take a drop (ed., of liquid) I separate it from the others and therefore for me there are no constraints"*, (*"non ci sono legami! Se io prendo una goccia (NdR, di liquido) la separo dalle altre e quindi per me non ci sono vincoli"*, the term 'constraint' shows up again). Another student replies *"in that drop there are bonds between particles"* (*"in quella goccia ci sono legami tra le particelle"*); another student says *"there are bonds, but those bonds are lighter, the particles are close but not attached to each other"* (*"ci sono legami, ma quei legami sono più lievi, le particelle sono vicine ma non attaccate"*); other similar remarks are made by students. At the end of the discussion, the teacher asks the first pupil if she has changed her mind after the discussion. She replies: *"yes, surely there are bonds, but they are weaker; the bond will never be the same as in solids"* (*"sì, sicuramente ci sono legami, ma sono più deboli; il legame non sarà mai uguale a quello di un solido"*).

The answers to the fourth question inform us that all, but two students agree that there are no constraints between helium particles in the gaseous state. The two students argue that *"In my opinion, although atoms are very far from each other, they are still bound"*, (*"Secondo me gli atomi pur essendo molto distanti fra loro sono comunque legati"*); *"There are constraints because atoms are a little bound together"* (*"Ci sono vincoli perché un minimo gli atomi sono legati tra loro"*). The students' justifications refer to the fact that the particles are not bound, they are far from each other and scattered, they are freely moving and the high temperature breaks the constraints. The discussion confirms the problems highlighted by the compilation of this WS: all students (except two pupils) agree in the belief that *"there are no bonds"* (*"non ci sono legami"*), *"the atoms are far from each other there is no bond that keeps them close or ordered"* (*"gli atomi sono distanti, non c'è legame che li tiene vicini o ordinati"*). A perplexed student states *"I have a doubt, it makes me think that there is some kind of bond; maybe very weak"* (*"ho un dubbio, mi viene da pensare che qualche legame ci sia; magari molto debole"*). The teacher intervenes in order to help her to better explain her thoughts and asks her: *"Do you think that this interaction acts at a distance, is it very weak?"*, The student says *"It acts at a distance"* (*"Agisce a distanza"*).

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
2	To understand the correlation between the values of melting and boiling temperatures of a given substance and the entity of the bonding forces existing between the constituent units of that substance.	- This WS facilitates the understanding of the link between melting and boiling temperatures and the entity of the interatomic bonding forces. - This WS consolidates the understanding of the relationship between macroscopic evidence and microscopic characteristics of a system.	None. Before delivering this WS, the teacher verified that the Kelvin scale had been well understood by the students.	None.
Outcomes of the answers provided by students and of the shared discussion				
Analysis of the answers to WS 2 indicates that most students understood the quantitative correlation between melting and boiling temperatures and the magnitude of bonding forces between particles: strong bonds need more energy to be broken than weak bonds. Two students state that the bond between He atoms is stronger than that between Ne atoms. A student converts temperatures from K to degrees Celsius, but then he gets confused while comparing them, as he assigns higher values to Helium because he neglects the negative sign. Another student calculates the difference between the boiling and melting temperatures of the two substances: since this difference is greater in the case of He, the student believes that the greatest bond forces occur between Helium atoms. During the discussion, the idea shared by the majority of students is that the bonds between Neon atoms are stronger because the melting and boiling temperatures of Neon are higher than those of Helium.				

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
3	To understand the correlation between the values of melting and boiling temperatures and the entity of the binding forces existing between the constituent units of a homologous series of substances.	This WS consolidates the knowledge acquired through WS 2, and allows students to formulate the first interpretative hypotheses. The discussion of the results reveals alternative conceptions.	- The lack of clarification of the meaning of Z. According to the teacher, this would facilitate the interpretation of the experimental data by the students - The teacher reports that the specification concerning the solidification pressure of He generates confusion and concur in diverting the students' attention from the learning objective of the WS. Therefore he suggests to cancel it, due to its non-fundamental character in this context.	To explain the meaning of Z. To cancel the note on the solidification pressure of Helium, which is misleading for students.
Outcomes of the answers provided by students and of the shared discussion				
The answers to WS 3 suggests that most students have correctly ordered the Noble gases according to the increasing entity of interatomic bond strength. Some students justify the proposed trend by saying that it goes along the increasing trend of the melting and boiling temperatures of substances. Someone justifies their choice by arguing that the growing trend of bond strength depends on the growing trend of Z. Finally, a student orders the noble gases based on the difference between the boiling and melting temperatures of each substance: the ratio behind this decision is that the smaller this difference, the smaller the entity of interatomic bond strength. This leads to a reversed order between He and Ne. This interpretation was already found in some answers to WS2. Its reiteration is perhaps due to the fact that WS 3 was awarded at the same time as WS 2, before opening the discussion on WS 2. Unfortunately, the organization of teaching activities was heavily influenced by the ongoing health emergency and the teacher was forced to assign multiple tasks at the same time, against the sequence schedule. In the end, the discussion allowed to summarize and consolidate the concept that the increasing melting and boiling temperatures of noble gases (in the order He, Ne, Ar, Kr, Xe and Rn) can be explained by the progressive increase of the entity of the interatomic bonding forces.				

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
4	To check Coulomb's law and understand its physical meaning.	The simulation was useful for consolidating the concept of electrostatic interaction and verifying the meaning of Coulomb's law, i.e. the influence of the 'charge' and 'distance between charges' on the entity of the interaction.	None	None
Outcomes of the answers provided by students and of the shared discussion				
In order to verify the students' understanding of the mathematical expression of Coulomb's law, students were invited to use a simulation that allows verifying how the interactions between electrical charges are affected by their distance, their sign and the entity of the charges themselves. The teacher followed the students during the simulation and while they were answering the questions listed in WS 4. According to the teacher, all students answer these questions correctly, without meeting serious obstacles. This exercise was effective and the IT tool represented a valid didactic support to consolidate concepts already learned in the physics course. According to the teacher, the purpose of this activity was achieved and was a valid preparatory step to the discussion of bonding between particles in terms of electrical attractions and repulsions, i.e. interaction between charged particles.				

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
5	To consolidate the concept of electron mobility. To build the notion of barycenter of negative and positive charges within a particle. To build the concept of dipole as a system wherein the barycenters of positive and negative charges do not coincide. To build the concept of instantaneous dipole as a consequence of electron mobility.	- Effectiveness of the simulation in reinforcing the idea that electrons are charges in endless motion, whose position varies moment by moment. - The comparison between different spatial distributions of electrons in the He atom, instant by instant, is a good support for the construction of the concept of symmetric and asymmetric charge distribution within the atom. This prepares students to understand the concept of instantaneous dipole.	The use of representations of the He atom to highlight the possibility of having asymmetric instantaneous distributions of electrons around the nucleus raised some problems. In fact, due to the small number of electrons involved, some students proposed two distinct, but equally asymmetrical, distributions of electrons within the He atom, in two subsequent instants. As a consequence, the aim of discussing systems wherein barycenters of positive and negative charges do not coincide was not achieved. The fourth question needs to be rephrased. In fact, several students misunderstood the request, as they proved unable to understand what 'charge distribution' meant. More in detail, charge symmetry was mistaken for neutrality, that is the parity of positive and negative charges; hence the choice of answering "symmetrical". The questions concerning the concepts of barycenter of electric charges and electric dipole also highlighted various critical issues. Due to the lack of coordination with the physics course, the students were not familiar with these concepts and this prevented them from answering autonomously to requests.	The replacement of the He atom with a Ne atom, with 10 electrons, may ease the representation of asymmetric distributions of negative charges. On the other hand, a high number of electrons might complicate the identification of the barycenter of negative charges. To overcome this problem, Neon might be mentioned in questions 1 and 2, whereas Helium might be mentioned in question 7, only. Rephrase question 4 so to make it more understandable to students. For example, the term "distributed" might be replaced with "positioned" or "located", so to lead students focusing on the spatial collocation and the relative positions of particles. This activity should imply the preparatory intervention of the physics teacher, in view of an integrated treatment of the concept of dipole by the two disciplines.

Outcomes of the answers provided by students and of the shared discussion

WS 5 was assigned as a homework. Before discussing the students' answers with the class, the teacher asked students whether they detected any inconsistency in the simulation they have viewed. It turned out that the simulation raised several questions to students: i) they were surprised to realise the mobility of nuclei, which was against their expectations; ii) some students noticed that electrons' orbits were not highlighted in the simulation. This led them to state that *"By following the trajectory of a single electron, the orbit could be imagined"*, (*"Seguendo la traiettoria di un singolo elettrone l'orbita la si poteva immaginare"*). The teacher ended this preamble by inviting students to look at the relative proportions of the nucleus vs. the atom, in the simulation: the nucleus is clearly misproportioned, as it occupies most part of the atomic volume. The analysis of the answers to WS 5 shows that most representations of the Helium atom, at the electron-nucleus level, in two subsequent instants made by students were correct. A couple of students did not represent the element Helium, but an atom with more than 2 electrons, like the one shown in the simulation. All students agreed that the position of the electrons changes with time, due to their mobility. Only a student did not justify this step correctly. Answering question 4 turned out to be rather problematic. Several students couldn't answer or they gave inconsistent or incomprehensible explanations: *"It is asymmetrical because they always follow the same orbits"*, (*"Asimmetrico perché seguono sempre le stesse orbite"*). Two students argued that the charge distribution within the atom could be either symmetrical and asymmetrical: *"It depends on the situations"*, (*"Dipende dalle situazioni"*). In this regard, the justification provided by a student was especially interesting: *"It is asymmetrical, because in our drawing they are asymmetrical. But, since they are in endless movement, they might at a given time, be symmetrical, but we do not know"*, (*"Asimmetrica, perché nel nostro disegno sono asimmetriche, ma dato che sono in continuo movimento potrebbero, in un certo periodo, essere simmetriche ma noi non lo sappiamo"*). On the other hand, some students associated an asymmetrical electric charge distribution to their representations, according to the expected result. In fact, an symmetrical charge distribution is proposed in the second part of WS 5. During the discussion, the teacher noticed that some students inconsistently connected a symmetrical charge distribution with the neutrality condition of the atom: they mixed up the two concepts, possibly due to the fact that Helium contains 2 electrons and 2 protons. The teacher suggested them to pay attention to the positions occupied by the electrons in the two aforementioned examples, instead of focusing on the charge balance; this indication seems to help them understand the distinction between the parity of positive and negative charges, an event that makes the atom neutral, and the mobility of electrons which may lead to the non coincidence of the barycenters of negative and positive charges in the atom. The fifth question, concerning the charge neutrality of the He atom, did not cause any problem: all students agreed that the atom is neutral because the negative and positive electric charges are equal in number. Many students were unable to answer to question 6, others answered unsatisfactorily and provided irrelevant justifications. After discussing this issue with the teacher, the students' doubts - concerning the possibility that the barycenter of negative charges varies moment by moment, due to the mobility of the electrons - were removed. Students were then further guided to think about the fact that asymmetric charge distributions within the Helium atom imply the non-coincidence of the barycenters of positive and negative charges. To the seventh question, concerning the symmetrical distribution of electric charges in the He atom, students answer according to the expectations. Both answers and justifications to questions 8 were overall acceptable: *"It is neutral, because the same number of particles (neutrons, protons, electrons) are present, so their charges cancel each other out"*, (*"Neutro, perché essendo presente lo stesso numero di particelle, (neutroni, protoni, elettroni), le loro cariche si annullano"*), or: *"It is neutral, because there are 2 protons and 2 electrons, so they cancel each other out"*, (*"Neutro, perché ci sono 2"*

protoni e 2 elettroni, quindi si annullano a vicenda”). Some students couldn’t answer to question 9, others answered according to the expectations, but they did not provide a justification. This question was discussed in the classroom and the correct motivation was shared with the class. The answer to question 10 raised some obstacles. In fact, some students could not answer, others gave wrong answers and justifications: *"Yes, because only the electrons move, the nucleus is stationary"*, (*“Sì, perché solo gli elettroni si muovono, il nucleo sta fermo”*), or: *"Yes because the nucleus of protons and neutrons rotates on itself in the same point, the electrons rotate on regular orbits"*, (*“Sì perché il nucleo di protoni e neutroni ruota su sé stesso nello stesso punto, gli elettroni ruotano su orbite regolari”*). Other students answered correctly and provided justifications such as: *"Sometimes they coincide, but not always"*, (*“A volte coincidono, non sempre però”*). After discussing this issue with the teacher, most students agreed on the fact that the barycenters of negative and positive charges in an atom do not always coincide. Question 11 raised some problems as well. These problems are likely due to the fact that the concept of electric dipole had not yet been discussed by the physics teacher. Students dealt with the notion of instantaneous dipole in the chemistry course, first.

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
6	To understand that constraints between the He and Ne atoms arise from the formation of temporary dipoles. Correlate the bond strength between atoms of noble gases with the number of electrons in each atom.	Students are led to think about the relation between electrons and bonds; in addition they are led to correlate the number of electrons in the atom with the strength of the interaction between instantaneous dipoles.	Several students found it difficult to represent the electronic distribution of atoms with more than two electrons (in this case that of the Ne atom). Question 2 is ambiguous and need to be rephrased: in fact, some students were led to think about bonds between He and Ne atoms, instead of considering the two substances separately.	Previous to this activity, the teacher need to assess the students' knowledge of the atomic layer model (requirement) and of the electron distribution within each layer. Question 2 must be rephrased in order to make it clearer, e.g. by proposing the two questions separately: • How do you explain the existence of bonds between He atoms? • How do you explain the existence of bonds between the Ne atoms?
Outcomes of the answers provided by students and of the shared discussion				
The representations of the He atom, at the electron nucleus level, task 1, were performed correctly by students. Conversely, the representations of Ne atoms showed some critical points: several students used three orbits and distributed a wrong number of electrons in the levels. During the related discussion with the class, the teacher drew the representations of both atoms on the tablet, with the assistance of the students. Few students answered autonomously to question 2, by stating that the constraints are consequent to the attraction between the instantaneous dipoles. In this regard, it is relevant that many students misunderstood the request; in fact, they thought of interactions between he and Ne atoms, instead of links beteeen eitherHe atoms or Ne atoms. After clarifying this point, the teacher discusses ths WS with the classroom by referring to the following concepts: • the various possible asymmetric distributions of electrons around the nuclei of Ne and He; • the non-coincidence of the barycenter of the positive and negative charges and the consequent raise of temporary dipoles. The shared conclusion was the identification of temporary dipoles as the probable cause of the constraints (bonds) between atoms. Students found difficult to answer to question 3, as well: they needed to be guided by the teacher who invited them to dwell on the fact that, the entity of the instantaneous dipoles increases with the number of electrons in the atom; consequently the entity of London's forces increases as well.				

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
7	To understand that the entity of the vaporization energy at constant P is related to the entity of the London dispersion forces (i.e. the bond energy between the noble gas atoms).	- To lead students think about the meaning of energetic parameters; to lead students identify the microscopic phenomena that justify the values of energetic parameters - The request made to students to propose a definition of "bonding energy".	Many students were unable to retrieve and exploit what they learnt from the last two activities (WS 5 and 6) and to contextualize them in the new situation proposed by WS 7. Most of them assigned the values of vaporization energies to each substance in a mechanical way, just following the order of noble gases in the Periodic Table. The results show that the students managed to correlate the amount of vaporization energy with the number of electrons, but were unable to conclude the reasoning, by correlating the number of electrons with the entity of the London dispersion forces. It is possible that this outcome is partly due to the ineffectiveness of distance learning which affects the teaching-learning schedule and penalizes interactions between the subjects.	In order to prevent the mechanical assignment of vaporization energy values to each substance, it is advisable to list the noble gases in a random order, using tables instead of graphs, so to favor the implementation of coherent reasoning.
Outcomes of the answers provided by students and of the shared discussion				
The analysis of the answers to WS 7 shows that all students associated vaporization energy values with their respective noble gases correctly. However, many of them provided unsatisfactory justification for their answer. Some students did not justify their choice, while most of them justified it by asserting that vaporization energy increases with the atomic number and, therefore, with the number of electrons in the atom. These statements are correct, but incomplete: in fact, any student proved able to link the conclusions of WS 6 with the examples of WS 7. In other words, no student was able to connect the increase in electrons' number with the magnitude of the London dispersion forces, responsible for the increase in vaporization energies. Some examples of student's answers are: "<i>In these substances the number of electrons changes (increases), it will be necessary to provide more energy</i>", ("<i>Nelle sostanze il numero di elettroni cambia (aumenta), bisognerà fornire più energia</i>"); "<i>The criterion I used is the quantity of electrons, the more they are, the more difficult and slow the state transition of a given substance</i>", ("<i>Il criterio che ho utilizzato è la quantità di elettroni, più ce ne sono più è difficile e lento il passaggio di stato di una determinata sostanza</i>"). The teacher reports that a student relied on the density of noble gases in order to carry				

out the assignment, without making any reference to previous activities. The students' answers concerning the definition of bonding energy were not very precise. Students understood that the bonding energy pertains to the interaction between atoms, but they mixed up the energy acquired or released by the system. Some examples of ambiguous answers are: *"It is the energy that is needed to create bonds between atoms"*, (*"È l'energia che serve per creare legami tra gli atomi"*); *"It is an energy that allows atoms to connect with each other"*, (*"È un'energia che permette agli atomi di collegarsi tra loro"*). A more pertinent answer is this: *"It is the energy needed to break a bond"* (*"È l'energia necessaria a rompere un legame"*), while a student provides the most comprehensive answer by stating that: *"It is the energy needed to break a bond and it is also the energy that is released when one form a bond"*, (*"È l'energia necessaria per rompere un legame ed è anche l'energia che si libera quando si forma un legame"*). During the debate, the teacher guided the students to think of the meaning of vaporization energy. Students focused their attention on the fact that it represents the energy that allows the transition from the liquid to the gaseous state and therefore it is the energy needed to break or weaken the bonds between the constituent units of the substances examined. Subsequently, the teacher encourages students to reflect on the role of energy in the case of the formation of a bond. Following this discussion, a student stated that *"If I have to supply energy to break the bond, I have to remove it to form the bond"*, (*"Se per rompere il legame devo fornire energia, per formare il legame devo toglierla"*). A student promptly stated that bonding energy is *"The energy that passes to the environment when a bond is formed"*, (*"L'energia che passa all'ambiente quando si forma un legame"*). In this way the class achieved the goal of sharing a correct and coherent definition of bonding energy.

WS N°	Learning objectives	Strengths	Critical issues	Future improvements
8	To consolidate the correlation between the entity of the London dispersion forces and the total number of electrons present in the elementary units of a substance.	- To highlight the correlation between vaporization energies, boiling temperatures and the entity of bond forces. - To stimulate student to mobilize their previously acquired knowledge.	As in the previous case, students tend to assign the values of vaporization energies and boiling temperatures mechanically, by following the order proposed by the text of the question (from H₂ to I₂). The comparison between all the proposed elementary substances confuses students' reasoning. The proposed activity was meant to be a consolidation activity. Unfortunately, too many uncertainties emerged. They highlighted the inadequate understanding of the concepts learned by students during previous activities. Once again, the limits of distance learning and the negative effects on learning outcomes come out.	- To list substances in random order. - To consider pair of substances in discussing the criterion to be applied
Outcomes of the answers provided by students and of the shared discussion				
The analysis of the answers to WS 8 shows that all students associated vaporization energy values with the listed substances correctly. However, the justifications provided by students highlighted various problems. Two students, albeit not mentioning London's forces specifically, wrote: <i>“High boiling temperatures and high vaporization energies indicate a strong bond between atoms. The strength of these bonds increases as Z grows, which is why I have ordered the elements in an increasing manner”</i>, (<i>“Alte temperature di ebollizione e alte energie di vaporizzazione indicano un forte legame tra gli atomi. La forza dei legami aumenta mano a mano che Z cresce, per questo ho ordinato gli elementi in maniera crescente”</i>). A student related the experimental data with the magnitude of the London forces and argued that: <i>“Increasing the number of electrons implies increasing the magnitude of δ^- and δ^+”</i>, (<i>“Aumentando il numero di elettroni coinvolti aumenta l'entità dei δ^- e δ^+”</i>). Two other students reported that their choice was based on the number of electrons, protons and neutrons. Finally, we remarked a student who justified his answer: <i>“By the atomic number, because I believe that for example H₂ has a double atomic number as compared to H and so on”</i>, (<i>“Per il numero atomico, perché credo che per esempio H₂ abbia il numero atomico doppio di H e così via”</i>). He erroneously				

extended the concept of atomic number, that is an atomic property, to the molecule; he therefore failed to realise that the number of electrons is doubled; finally, he did not compare the elements of the series.

In the classroom, the teacher took note of the difficulties met by students, he invited them to make a comparison between just two substances in the list and asked provocative questions such as: "*Why is the bond between F_2 molecules more intense than between H_2 molecules?*". A student replied that she had thought about the atomic number, because there are more electrons and protons that attract more each other. However, she could not clarify which entities she was referring to while thinking about attraction. Another student stated that there are more electrons in the fluorine molecule and therefore the instantaneous dipoles are stronger. After further discussion, the class got to the shared conclusion that - in a homologous series of substances - the intensity of London's forces increases as the number of electrons increases.

5.4 Concluding remarks

At the end of this thesis work, we wish to formulate some remarks of epistemological-conceptual and didactic nature, which summarize some issues discussed in more details in chapters 2, 3 and 4 of this thesis.

- The concept of bond and its descriptive models belong to different conceptual levels. **The concept of bond is placed upstream of its descriptive models:** it has its roots in the concept of chemical affinity and helps to justify the persistence and stability of chemical substances and / or physical states under defined conditions of temperature and pressure. The concept of bond - understood as the interaction between the constituent particles of substances - runs through the history of chemistry from Dalton onwards. Along this historical path, it has been declined by means of various bonding models, depending on the development of the chemical and physical knowledge typical of each historical period. It is relevant to remark that **each of these bonding models corresponds to different definitions of the bond itself**. For example, according to the Lewis theory the bond is described as an electronic doublet shared between two atoms, whereas in the quantum description the bond is a quantum effect, expressed mathematically by the linear combination of atomic orbitals and it can be polycentric. Some models and bonding theories are now definitively outdated and have been abandoned (e.g. the Berzelius model). Other models coexist and are still used in relation to various research questions: for example, the Lewis model is widely used in the description and design of organic syntheses, thanks to its heuristic value; quantum models are instead applied to the description of the molecular structure and to the interpretation of spectroscopic data.

In the didactic practice, the conceptual level is rarely distinguished from the modeling one: **the bond is never defined as such, it is instead described through its models**. This generates various problems, since: i) the explanatory needs that the concept of bond is called upon to satisfy are not discussed; ii) the overlap of the concept with its models makes the use of different bonding models difficult to understand: the student may in fact wonder which is the authentic definition of bond; only the distinction between concept and models makes the evolution of bonding models and the consequent change in the definition of bond from one model to another, understandable and logically acceptable; iii) the link between reality and its descriptive and interpretive models is not made explicit, with the result that students are induced to mix up the empirical and interpretative levels.

We attempt to take these problems into account, by designing our teaching sequence as **a succession of interpretive models**, whose design is stimulated by the need **to find suitable interpretations for a variety of empirical phenomena**.

For this reason, it was decided to adopt the examination of some macroscopic properties of various materials as the starting point: it is the wide range of properties exhibited by various substances (or combinations of substances) that **stimulates the search for interpretive models** and justifies the need for a range of models, which aim at interpreting the different chemical-physical properties of substances.

Furthermore, in our didactic sequence, it is precisely the **critique of previous models** that urges the development of new models whenever a bond model is ineffective for interpreting a given phenomenology: this allows highlighting both the **model character** that characterizes

any operational description of the bond, and the **limits of the model** in terms of its field of existence and applicability.

For example, our teaching sequence introduces the ionic bond model after verifying the inadequacy of the covalent bond model for interpreting the macroscopic properties of ionic compounds; similarly, the metallic bond model is designed after verifying the ineffectiveness of the covalent and ionic bond models in justifying the peculiar properties of metallic substances.

- Educational research (Cooper et al. 2015; Ghibaudi and Branchini, 2021; Levy Nahum et al. 2007) indicates that students tend to have a dichotomous view of intramolecular interactions and chemical bonds, and are unable to recognize the fact that all kinds of interatomic interactions have a **common electrostatic basis**. Such dichotomous view is ascribed to two main factors: i) a **didactic practice** that does not highlight the elements of continuity and contiguity of the two concepts and treats these concepts in sharply separated contexts (the discussion of physical states for inter-molecular bonds, reactivity for chemical bonds, respectively); ii) a **terminology** that emphasize the differences between the two bonding phenomena, to the point that inter-molecular bonds are generally designated as *interactions*, whereas the term *bond* is used only for covalent¹⁶, ionic or metallic interactions. This leads students to think that interactions are physically distinct from bonds. Epistemological reflection (Hendry 2008) indicates that interatomic interactions can be treated under two distinct perspectives, the physical and the chemical one. The physical perspective focuses on the **energy aspects** and differentiates these interactions on the basis of the binding energy. This perspective has the advantage of underlining the elements of continuity between the various types of interatomic interaction, but it has the limit of not bringing out the different meaning that chemical bonds and inter-molecular interactions have for chemistry. According to Hendry, the chemical perspective focuses on **structural aspects**. It is only this latter perspective that allows identifying the constituent units of substances (molecules, lattices), distinguishing them from their surroundings, i.e. distinguishing between an internal environment (intra-molecular or intra-reticular) and an external one (e.g., the relationship amongst the molecules or the constituent units of a substance and of the medium in which the substance is dispersed), and correlating them to a specific reactivity. Furthermore, this perspective - which clearly distinguishes inter-molecular interactions from chemical bonds - allows us **to set out a differentiation criterion for chemical and physical transformations**: in the former case, chemical bonds are broken and formed; in the latter, only intermolecular bonds are involved. The terminological problem mentioned above could be expressed in these terms: is it correct to distinguish between intermolecular *interactions* and chemical *bonds*, reserving the term *bond* to the latter? The consequences of the use of this terminology on students' understanding of interatomic interactions show that the question is not purely formal. A broader question could be: is it correct to treat inter-atomic interactions according to two clearly separated classes? Here are some arguments for and against this choice:
 - i) By restricting the term *interaction* to inter-molecular bonds and by using the term *bond* to intramolecular, ionic and metallic substances, one feeds the misconception that these are

¹⁶ With the exception of the hydrogen bridge bond

radically distinct physical phenomena, and overlooks the fact that both classes involve interactions between charged particles (electrons and nuclei).

- ii) However, the absence of differentiation between kinds of interaction would be equally misleading, as it would drop the (microscopic) criterion that allows classifying changes as chemical or physical, depending on the type of interaction involved in the transformation itself.
- iii) An important element of differentiation is represented by the type of perturbation that each class of interactions entails: the formation of chemical bonds involves the modification of the outer electron shell of the bonded atoms, a modification that remains as long as the corresponding substance remains. Conversely, the formation of inter-molecular interactions leaves the electronic configuration of the atoms unchanged and implies transient interactions. Which terminology could favor the understanding of both the continuity and the discontinuity factors between the two classes of interactions? Suggestions from the literature lead to advise against the use of different terms: it is then matter of choosing between the terms *interaction* and *bond*. In our teaching sequence we opted for the latter term, and we choose to designate all different types of interatomic interactions as **bonds**. However, the term *bond* needs to be further qualified, in order to identify the two aforementioned kinds of interaction which – we would like to stress it - are associated to distinct types of transformation. We believe that the qualification of *intermolecular* vs. *intramolecular* has to be avoided, primarily because not all 'chemical' bonds involve the formation of molecules (i.e., not all substances are molecular): hence, not all chemical bonds are *intramolecular*. Some texts differentiate between chemical bonds and physical bonds: it seems to us that this term is misleading, as it seems to suggest that chemical bonds have no physical character. A better option is adopted by some texts, which mention *primary and secondary bonds*, to designate chemical bonds and inter-molecular interactions, respectively. These two adjectives have the advantage of avoiding a too clear choice of side and leave open the possibility that secondary interactions may play a role in chemically relevant processes, as we learn from supramolecular chemistry.

- After discussing the terminological aspects, let us go back to those aspects that are shared by all different types of interatomic interactions, i.e. the **electrostatic aspects** and the **energetic aspects**. Concerning the first point, it is clear that the knowledge of the atomic structure in terms of subatomic structure (electrons, nuclei) is a necessary premise for approaching the bonding notion. This issue helps clarifying the connection between the structure of matter and the concept of bond, by discussing the character of electrons as negatively charged particles, in endless motion, whereas atomic nuclei are positively charged. It is only through the discussion of all the implications of the endless motion of electrons that students may be led to understand inter-molecular interactions. On the other hand, **the electrostatic nature of the interactions between electrons and nuclei serves as a unifying framework for all interatomic interactions**. Regarding the **energy aspects**, their treatment is fundamental for several reasons. Energy considerations serve: i) to justify the formation of bonds; ii) to clarify the different stability of the different types of interatomic interactions, by highlighting the quantitative relationships existing between them; iii) to underline the continuum of bonding forces, an aspect whose didactic importance is emphasized by various studies available in the literature (Dhindsa and Treagust 2014; Levy Nahum et al. 2008).

For all these reasons, our teaching sequence was based on following choices:

- i) **Chemical bonds and inter-molecular interactions are treated within a unitary conceptual framework**, according to a non-linear and unconventional path that alternates these two kinds of interactions. Along this path, various **energy data** are discussed by relating them to the stability of the systems gradually taken into consideration. This choice is aimed at **discouraging the above-discussed dichotomous view of bonds and to highlight the continuum of bonding forces**.
- ii) The bonding notion is first introduced through **the discussion of the physical states of noble gases, which allow introducing the London dispersion forces**. These affect all types of substances and therefore represent the most general type of interatomic interaction. By taking the properties of monoatomic substances as the starting point, the conceptual complications relating to molecular systems, where chemical bonds and inter-molecular interactions are simultaneously present, are avoided. This choice allows discussing thoroughly the **implications relating to the endless motion of electrons around nuclei, which are the necessary premise for building the concept of electric dipole**. The concept of dipole is a serious learning obstacle which is easily misunderstood by students, who often represent dipoles as electrically charged species. **The activities of the sequence aim at highlighting the fact that a dipole is an electrically neutral system, in which the barycenters of positive and negative charges do not coincide**. The discussion of the properties of noble gases allows introducing the possibility that, by virtue of the electrons' motion, the barycenter of negative charges changes continuously over time, thus generating instantaneous dipoles.
- iii) The use of Lennard-Jones graphs allows inscribing the formation/rupture of any interatomic interaction within a unifying logical framework. It helps to understand that equilibrium states (e.g., the formation of a molecule, the stabilization of a physical state, the dissolution of a solute in a solvent, etc.) is the result of a balance between opposite factors (e.g. attractive and repulsive forces) that bring the system into a condition of greater energy stability as compared to its isolated components.

Finally, we'd like to mention that a recent study conducted by Pazinato et al. (Pazinato et al. 2021) confirms that meaningful learning of the concept of bonding is achieved whenever the teaching approach takes into account the following three aspects:

- Emphasis on the energetic factors underlying the formation of bonds.
- Use of the electrostatic model to elucidate and justify the nature of all interatomic interactions.
- Macroscopic properties of substances are linked to bonding models that can justify them.

This teaching sequence includes all of these aspects.

To conclude, we wish to underline two purely didactic aspects:

- The choice of **avoiding quantum descriptions of bonding**, despite their greater interpretive effectiveness, is dictated by the desire to propose intelligible models to students attending a school level that is not yet specialized. The didactic sequence **privileges the construction of meanings to the memorization of contents**. We believe, in agreement with various scholars (Bent 1984; Dhindsa and Treagust 2014; Joki et al. 2015; Pauling 1983) that the description of the bond in terms of electrostatic interactions (and in particular the Lewis model) represents a didactically consistent choice, beyond the explanatory limits of historically outdated models.

- The **choice to use a constructivist-inspired approach, which relies on the use of worksheets and 'problem situations'** able to guide students in achieving the learning objectives, aims at favoring the active construction of concepts by students. Each worksheet aims at building a specific concept or to reinforce it. Students are actively involved in learning; the questions in the worksheets stimulate the application of previously acquired knowledge to new practical situations. The results of the survey discussed in Chapter 1 confirm the need to adopt teaching practices that promote reasoning skills and make students active subjects in the learning process.

The many limitations imposed by the pandemic have significantly changed the initial design of this PhD project. The impossibility of extensive experimentation hampered the critical review and remodelling the teaching sequence, based on the results obtained in the classroom. This work will need further extensive review, especially as regards to the following aspects: i) further discussions on conceptually critical issues; ii) acknowledgment of the results of the classroom experimentation, which will highlight critical issues and strengths; iii) a refinement of the teaching schedule according to which this sequence can be administered to students, in order to make it fully compatible with the school timing. The time scheduling of this teaching sequence was in fact neglected to favor, in the first instance, its conceptual architecture. For these reasons, the present teaching sequence is to be considered an ongoing product, which requires to be optimized both in its logical steps and in the administration schedule.

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Appendix 1

QUESTIONNAIRE FOR THE DETECTION OF INITIAL CONCEPTIONS

1) A pot full of water has been boiling for about an hour. What are the bubbles rising to the surface made of?

- a) Air b) Oxygen c) Water vapor d) A mixture of oxygen and hydrogen

Justify your answer:

Represents the phenomenon by means of the particle model:

Representation of boiling water using the particle model

2) A sulfur sample has the following properties:

- I. It's fragile
- II. It melts at 115°C



Which of the above properties belong to a single sulfur atom obtained from the sample?

- 1. Properties I and II
- 2. Only property I
- 3. Only property II
- 4. None of them

Justify your answer:

- 3) Crystals of iodine (I_2) placed in a hermetically sealed flask are weighed on a balance. Immediately thereafter, the flask is heated and purple vapors appear inside it (see figure below). Then, the mass of iodine contained in the flask is again determined by weighing.



In your opinion, the mass of the iodine sample:

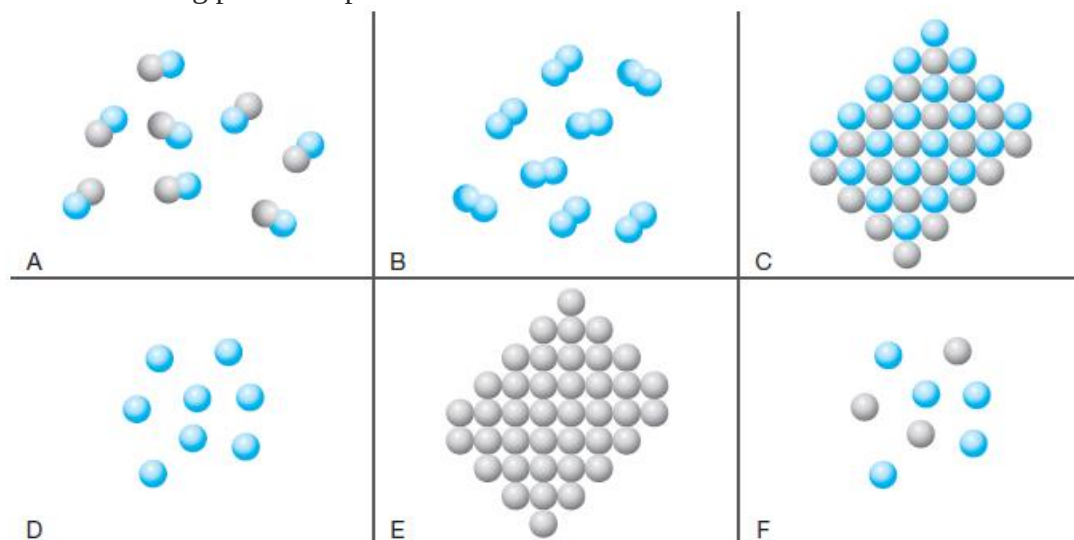
1. increased after warming up
2. decreased after warming up
3. remained unchanged after warming up
4. it is not possible to answer

Justify your answer by representing the iodine (I_2) contained in the flask before and after heating, by using the particle model:

Before warming up

After warming up

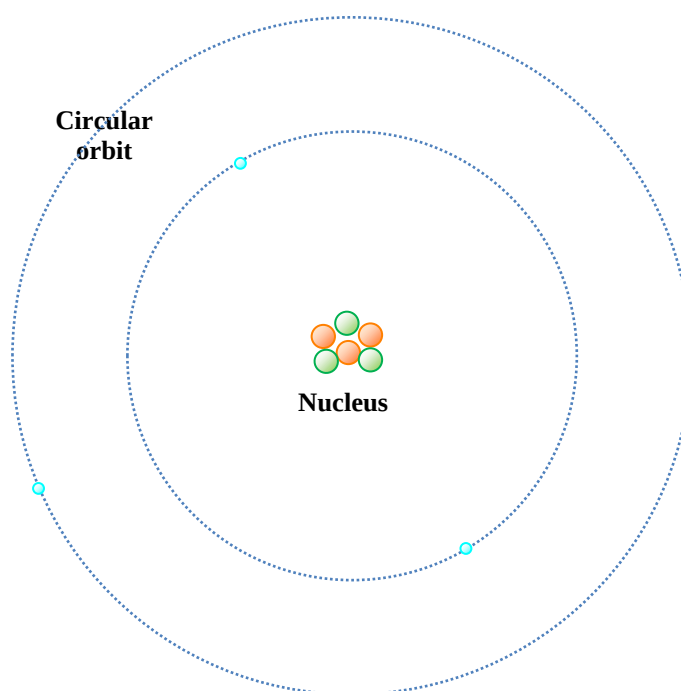
4) Look at the following particle representations of matter:



Which drawing (s) represent a compound substance, a simple substance, a mixture of simple substances?
Answer by crossing the boxes in the table:

A compound substance	A	B	C	D	E	F
A simple substance	A	B	C	D	E	F
A mixture of simple substances?	A	B	C	D	E	F

5) Look at the following representation of a **layered atomic model** and answer **True or False** to the statements below, by justifying your answer:



- It represents a neutral atom
 - The nuclear charge is +6
 - Electronic charge is 0
 - The electrons represented in the drawing are meant to be stationary
 - The mass of the atom is almost equal to the mass of the nucleus
 - There is a lot of empty space between nucleus and electrons
 - The distance between the nucleus and the electrons shown in the figure is represented correctly
 - It refers to a compound
 - The mass number is 6
 - It is a lithium atom
- 6) Two liquids, water and alcohol, are layered in a flask and brought to volume. Since water and alcohol are miscible, the alcohol should be made flow very slowly along the wall of the container. The flask is then placed on a balance in order to measure the mass of the system (Figure 1). Then, the content is stirred to mix the two liquids. After mixing, a solution is obtained: you will notice that its volume has decreased. The system is placed on the balance again and its mass is measured again you will notice that it is unchanged (Figure 2).

Figure 1
Total volume =
500 mL
mass = 324.3g



Figure 2
Total volume
<500 mL
mass = 324.3g



A. In your opinion, why did the volume decrease after mixing the two liquids?

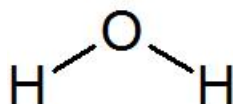
Try to represent the contents of the flask as it appears in Figure 1 and Figure 2, by using the particle model.

Mixed water and alcohol

Layered water and alcohol

- B. In your opinion, what does it change in the system made by water and alcohol particles, before and after mixing?
-

- 7) The following image represents a model of a water molecule, which is made up of one oxygen atom (O) and two hydrogen atoms (H):



- What do you think holds the three atoms in the water molecule together?
-
-

- 8) There are millions of chemical compounds, but only a few dozen elements. How can you rationally justify this evidence?
-
-

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