Trace retrieval for business process operational support

Bridging the gap between molecular scale simulations and environmental scenarios.

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Concept

The scope of this contribution is to review and put in perspective the relevance of molecular simulation techniques in environmental policy- and decision-making, with a focus on materials and materials-molecules interactiuons. Many solutions to environmental and energy issues require the deployment of technical strategies whose design is based on detailed chemical information on individual molecules and complex reaction systems. While in the past most of this information was derived from experiments, molecular simulations are increasingly used today in the prediction of molecular properties and chemical systems dynamics.

Motivations and Objectives

The apparently distant fields of molecular scale simulations and environmental simulations aimed at practical decision- and policy-making are increasingly mutually interacting. Simulations concerning materials and the interaction of materials with molecules are often involved. This work reviews these points of contact from a technical and methodological perspective.

Results and Discussion

The use of simulated chemical data in the solution of complex environmental problems can take different routes. In some cases, when the relationship between molecular properties and environmental dynamics is well understood, simulation substitutes experiments allowing the fast and efficient production of chemical data on large families of new compounds and systems [1].

In other cases, molecular simulations are used to derive information on complex systems on which experiments are difficult or impossible to run. This is the case for example of the prediction of the fate of pollutants in the atmosphere and in soils [2]. Multi-scale simulations provide the tools for such predictions.

A third and very powerful type of usage of molecular simulation in environmental studies is based on the production of calculated boundary conditions to environmental and technological problems [3]. Both calculated and experimental molecular data can in fact be used to define limiting conditions of natural or artificial systems. Predicted boundary conditions are essential in forecasting realistic technological and environmental scenarios, from which environmental and research policies are often derived.

Finally, our study reviews the maturity of the field of materials design for environmental and energy applications (an example in [4]) and the increasing extent to which these simulation technologies provide practical materials design solutions in the field of energy and the environment.

The overall goal of the study is not only to review the technical achievements obtained in the field, but also to highlight and analyze the methodologies adopted to translate molecular scale simulations into policy- and decision-making scenarios and to identify the bottlenecks in this process.

References

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