Prediction uncertainty of density functional approximations for properties of crystals with cubic symmetry

Supplementary Material

Pascal Pernot,[*,†,‡] Bartolomeo Civalleri,[¶] Davide Presti,[§] and Andreas Savin[‖,⊥]

CNRS, UMR8000, Laboratoire de Chimie Physique, F-91405 Orsay, France, Univ. Paris-Sud, UMR000, Laboratoire de Chimie Physique, F-91405 Orsay, France, Department of Chemistry and NIS Center, University of Torino, Via P. Giuria 7, I-10125 Torino, Italy, Department of Chemical and Geological Sciences, University of Modena and Reggio-Emilia, Via Campi 183, I-41125 Modena, Italy, CNRS, UMR7616, Laboratoire de Chimie Théorique, F-75005 Paris, France, and UPMC Univ Paris 06, UMR7616, Laboratoire de Chimie Théorique, F-75005 Paris, France

E-mail: pascal.pernot@u-psud.fr

[*]To whom correspondence should be addressed

[†]CNRS, UMR8000, Laboratoire de Chimie Physique, F-91405 Orsay, France

[‡]Univ. Paris-Sud, UMR000, Laboratoire de Chimie Physique, F-91405 Orsay, France

[¶]Department of Chemistry and NIS Center, University of Torino, Via P. Giuria 7, I-10125 Torino, Italy

[§]Department of Chemical and Geological Sciences, University of Modena and Reggio-Emilia, Via Campi 183, I-41125 Modena, Italy

[‖]CNRS, UMR7616, Laboratoire de Chimie Théorique, F-75005 Paris, France

[⊥]UPMC Univ Paris 06, UMR7616, Laboratoire de Chimie Théorique, F-75005 Paris, France

List of Tables

We provide here tables of all the data used in the companion paper and tables of the coefficients to estimate the corrected values and prediction uncertainties of the studied methods.

Validation data. Tables 1-6.

Reference data were collected for the following crystals (*Strukturbericht* designation[1] in parentheses): 22 semiconductors, also present in the SC40 data set[2], namely : C(A4), Si(A4), Ge(A4), SiC(B3), BN(B3), BP(B3), BAs(B3), AlP(B3), AlAs(B3), AlSb(B3), GaN(B3), GaN(B4), GaP(B3), GaAs(B3), GaSb((B3), InP(B3), InAs(B3), InSb(B3), ZnS(B3), ZnSe(B3), ZnTe(B3), CdTe(B3), MgS(B1); 4 alkali halides: LiF(B1), LiCl(B1), NaF(B1) and NaCl(B1); and, two oxides: MgO(B1), $SrTiO_3$($E2_1$).

The reference dataset includes: experimental lattice constant values corrected for the zero-point anharmonic expansion, as reported in Ref.[3]; experimental bulk modulus values, taken from Refs.[4–7], and low temperature (below 77 K) experimental (fundamental) band gap values[2,5,8,9].

For bulk modulus, we referred to low temperature data[4–6], if available, and, when possible, the zero-point anharmonic expansion correction has been included from Ref[6]. The band gaps considered cover two orders of magnitude, between ≈0.2 and ≈12 eV.

Validation data. Tables 7-10.

A set of 9 system has been set aside for validation purpose. These systems have been chosen on the basis that we did find reference values for band gaps and lattice constants, but none for bulk moduli: AlN(B3), CdS(B3), CdSe(B3), MgSe(B1), MgTe(B1), BaS(B1), BaSe(B1), BaTe(B1), and LiH(B1).

Propriety and uncertainty prediction. Tables 11-13.

For the estimation of a new value of a property knowing a calculated value c_s (for a system not in the benchmark set), the prediction model and prediction variance corre-

sponding to the chosen DFA are[10]

$$p(c_s) = a + bc_s \tag{1}$$

$$u_p^2(c_s) = u_f^2(c_s) + d^2 \tag{2}$$

$$u_{f_m}^2(c_s) = u^2(a) + u^2(b)c_s^2 + 2u(a,b)c_s. \tag{3}$$

For the comparison of a model prediction with reference data, or the prediction of an experimental result, this variance has to be further combined with the corresponding reference/experimental data uncertainty

$$u^2(c_s) = u_p^2(c_s) + u_s^2. \tag{4}$$

References

(1) *Strukturbericht* designation is taken from the Crystal Lattice Structures web page: http://cst-www.nrl.navy.mil/lattice/struk/index.html.

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Table 1: Reference data for lattice constants (Å).

System	Symmetry	Exp.	HF	LDA	PBE	PBEsol	B97	B3LYP	PBE0	PBEsol0	HSE06
C	A4	3.555	3.555	3.534	3.575	3.557	3.577	3.573	3.549	3.537	3.549
Si	A4	5.422	5.501	5.410	5.479	5.442	5.494	5.495	5.443	5.420	5.448
Ge	A4	5.644	5.736	5.639	5.778	5.696	5.764	5.790	5.694	5.644	5.702
SiC	B3	4.348	4.390	4.357	4.406	4.383	4.395	4.403	4.375	4.361	4.377
BN	B3	3.592	3.598	3.579	3.623	3.604	3.613	3.617	3.595	3.583	3.596
BP	B3	4.527	4.591	4.508	4.564	4.537	4.584	4.579	4.538	4.521	4.539
BAs	B3	4.764	4.833	4.745	4.823	4.782	4.833	4.838	4.784	4.758	4.787
AlP	B3	5.450	5.521	5.429	5.503	5.465	5.504	5.514	5.468	5.443	5.471
AlAs	B3	5.649	5.734	5.623	5.722	5.670	5.713	5.731	5.677	5.643	5.681
AlSb	B3	6.126	6.237	6.092	6.205	6.141	6.198	6.225	6.155	6.113	6.161
GaN	B3	4.523	4.513	4.477	4.569	4.520	4.547	4.559	4.514	4.483	4.517
GaP	B3	5.441	5.560	5.428	5.540	5.476	5.547	5.561	5.490	5.449	5.495
GaAs	B3	5.641	5.762	5.626	5.770	5.687	5.762	5.786	5.701	5.648	5.708
GaSb	B3	6.086	6.217	6.043	6.210	6.109	6.201	6.231	6.132	6.071	6.141
InP	B3	5.858	5.988	5.845	5.972	5.894	5.971	5.999	5.909	5.860	5.915
InAs	B3	6.048	6.178	6.039	6.196	6.100	6.179	6.215	6.111	6.051	6.120
InSb	B3	6.473	6.611	6.433	6.610	6.502	6.597	6.638	6.523	6.454	6.533
ZnS	B3	5.399	5.578	5.338	5.484	5.402	5.509	5.520	5.449	5.393	5.452
ZnSe	B3	5.658	5.852	5.593	5.758	5.665	5.775	5.799	5.713	5.648	5.718
ZnTe	B3	6.079	6.340	6.023	6.206	6.100	6.231	6.264	6.161	6.091	6.167
CdTe	B3	6.470	6.755	6.422	6.625	6.500	6.644	6.681	6.564	6.481	6.571
MgS	B1	5.612	5.734	5.600	5.702	5.656	5.703	5.709	5.667	5.635	5.669
LiF	B1	3.974	3.996	3.906	4.060	4.000	4.044	4.023	4.004	3.960	4.005
LiCl	B1	5.072	5.271	4.977	5.158	5.076	5.187	5.190	5.120	5.063	5.124
NaF	B1	4.570	4.615	4.486	4.673	4.605	4.649	4.631	4.620	4.568	4.621
NaCl	B1	5.565	5.781	5.481	5.703	5.613	5.703	5.708	5.658	5.591	5.660
MgO	B1	4.188	4.184	4.162	4.256	4.218	4.241	4.232	4.207	4.177	4.209
SrTiO3	E21	3.900	3.911	3.865	3.946	3.902	3.931	3.937	3.902	3.830	3.904

Table 2: Reference data for lattice constants (Å), continued.

System	Symmetry	Exp.	HSEsol	HISS	RSHXLDA	wB97	wB97X	LC-wPBE	LC-wPBEsol	M06-L	M06
C	A4	3.555	3.538	3.529	3.531	3.565	3.560	3.538	3.512	3.554	3.548
Si	A4	5.422	5.424	5.424	5.404	5.427	5.436	5.392	5.373	5.426	5.453
Ge	A4	5.644	5.650	5.655	5.587	5.648	5.671	5.588	5.532	5.751	5.709
SiC	B3	4.348	4.361	4.352	4.348	4.381	4.378	4.352	4.322	4.353	4.365
BN	B3	3.592	3.583	3.578	3.581	3.620	3.610	3.589	3.563	3.598	3.600
BP	B3	4.527	4.522	4.517	4.514	4.548	4.550	4.509	4.485	4.532	4.549
BAs	B3	4.764	4.760	4.758	4.738	4.786	4.793	4.735	4.703	4.799	4.796
AlP	B3	5.450	5.445	5.446	5.432	5.447	5.461	5.422	5.393	5.441	5.477
AlAs	B3	5.649	5.646	5.652	5.618	5.664	5.674	5.616	5.578	5.685	5.676
AlSb	B3	6.126	6.118	6.128	6.087	6.134	6.148	6.072	6.035	6.182	6.171
GaN	B3	4.523	4.485	4.481	4.460	4.518	4.517	4.471	4.422	4.540	4.508
GaP	B3	5.441	5.453	5.460	5.420	5.449	5.476	5.415	5.374	5.506	5.503
GaAs	B3	5.641	5.654	5.664	5.600	5.659	5.683	5.602	5.547	5.750	5.705
GaSb	B3	6.086	6.077	6.094	6.019	6.079	6.107	6.012	5.958	6.210	6.149
InP	B3	5.858	5.865	5.872	5.830	5.849	5.885	5.812	5.769	5.948	5.931
InAs	B3	6.048	6.058	6.069	6.005	6.057	6.086	5.991	5.936	6.201	6.134
InSb	B3	6.473	6.462	6.479	6.402	6.453	6.489	6.384	6.327	6.646	6.563
ZnS	B3	5.399	5.396	5.428	5.385	5.430	5.449	5.385	5.345	5.462	5.438
ZnSe	B3	5.658	5.655	5.688	5.633	5.704	5.717	5.631	5.583	5.759	5.708
ZnTe	B3	6.079	6.095	6.135	6.073	6.149	6.171	6.055	6.011	6.239	6.187
CdTe	B3	6.470	6.487	6.529	6.469	6.539	6.565	6.448	6.396	6.703	6.600
MgS	B1	5.612	5.637	5.648	5.642	5.656	5.670	5.631	5.597	4.188	4.228
LiF	B1	3.974	3.961	3.991	4.004	4.038	4.042	4.021	3.958	5.616	5.652
LiCl	B1	5.072	5.065	5.103	5.151	5.156	5.206	5.090	5.053	3.981	4.051
NaF	B1	4.570	4.570	4.608	4.605	4.600	4.610	4.636	4.561	5.174	5.244
NaCl	B1	5.565	5.595	5.637	5.659	5.626	5.666	5.629	5.566	4.608	4.608
MgO	B1	4.188	4.178	4.190	4.183	4.240	4.228	4.201	4.153	5.699	5.757
SrTiO3	E21	3.900	3.874	3.884	3.888	3.927	3.920	3.889	3.853	3.930	3.915

Table 3: Reference data for bulk modulus (GPa).

System	Symmetry	Exp.	HF	LDA	PBE	PBEsol	B97	B3LYP	PBE0	PBEsol0	HSE06
C	A4	455.9	498.5	467.5	431.8	449.2	439.7	440.7	469.6	480.2	468.2
Si	A4	101.3	108.6	99.4	90.0	95.1	90.7	90.9	100.9	104.1	99.6
Ge	A4	79.4	85.2	74.8	61.5	65.6	66.9	61.5	75.4	80.9	73.5
SiC	B3	229.1	247.8	231.7	214.9	224.5	225.8	219.0	234.8	240.6	233.3
BN	B3	410.2	436.4	408.9	377.7	391.3	396.0	390.4	409.6	418.4	408.7
BP	B3	168.0	182.1	180.0	165.5	173.4	164.8	164.7	179.5	184.3	178.4
BAs	B3	151.1	151.6	148.0	132.1	141.0	134.3	132.7	147.0	152.7	145.7
AlP	B3	87.4	100.0	94.2	85.6	90.5	91.4	87.2	95.1	98.1	94.3
AlAs	B3	75.0	88.0	82.8	73.3	78.7	78.7	75.1	82.8	86.2	81.9
AlSb	B3	58.2	65.9	62.9	54.8	59.6	59.1	55.7	62.2	65.5	61.3
GaN	B3	213.7	215.8	197.4	166.9	182.8	180.9	177.7	194.4	205.5	193.0
GaP	B3	92.3	94.5	91.5	77.9	85.9	83.4	78.7	90.1	95.2	88.8
GaAs	B3	78.0	80.1	74.5	62.2	69.5	66.7	62.4	73.7	78.9	72.2
GaSb	B3	57.9	62.5	60.4	46.4	54.5	52.5	49.3	57.9	62.7	57.9
InP	B3	72.0	76.1	73.0	60.7	68.2	66.8	61.7	71.8	76.6	70.6
InAs	B3	58.6	66.0	61.4	49.5	56.7	54.7	49.1	60.2	65.3	58.9
InSb	B3	46.1	53.4	50.7	40.3	46.1	45.2	39.2	48.7	53.0	47.5
ZnS	B3	75.0	71.6	86.3	70.7	79.1	71.0	69.8	77.6	83.4	77.0
ZnSe	B3	65.9	59.0	72.8	58.1	66.7	60.3	56.6	65.0	70.4	64.3
ZnTe	B3	52.8	44.0	56.6	44.1	51.6	44.6	42.4	49.9	54.9	49.2
CdTe	B3	45.0	37.1	47.4	35.9	42.3	38.1	35.3	41.0	45.7	40.4
MgS	B1	78.9	61.8	64.9	58.0	60.9	60.9	59.1	62.4	64.2	62.2
LiF	B1	76.3	78.4	90.2	70.4	75.7	73.7	75.7	76.5	81.2	76.4
LiCl	B1	38.2	30.0	41.8	32.4	36.1	32.1	32.0	34.6	37.5	34.5
NaF	B1	53.1	53.4	68.5	51.6	55.2	53.2	54.4	54.5	57.5	54.5
NaCl	B1	27.6	22.7	33.8	24.6	26.9	24.5	24.5	26.0	27.9	25.9
MgO	B1	169.8	183.4	179.2	158.5	165.0	159.6	165.9	173.2	178.6	172.9
SrTiO3	E21	179.0	215.9	203.8	171.3	187.2	185.8	184.5	196.0	208.0	195.3

Table 4: Reference data for bulk modulus (GPa), continued.

System	Symmetry	Exp.	HSEsol	HISS	RSHXLDA	wB97	wB97X	LC-wPBE	LC-wPBEsol	M06-L	M06
C	A4	455.9	479.3	498.3	488.8	464.6	461.6	493.3	528.1	452.9	459.0
Si	A4	101.3	102.9	106.8	113.2	113.6	109.5	118.3	126.0	101.4	98.4
Ge	A4	79.4	79.1	81.7	92.7	92.6	87.2	97.8	107.7	62.9	68.7
SiC	B3	229.1	239.4	248.9	249.9	239.6	240.3	255.9	272.4	227.5	228.4
BN	B3	410.2	417.9	431.9	422.9	394.6	401.3	426.7	453.7	395.8	397.2
BP	B3	168.0	183.4	189.1	189.4	184.9	179.4	196.3	205.9	177.0	171.6
BAs	B3	151.1	151.7	156.3	161.4	155.5	151.3	167.4	178.3	137.2	139.3
AlP	B3	87.4	97.4	100.8	105.1	107.6	103.4	109.5	114.7	95.1	93.4
AlAs	B3	75.0	85.4	87.6	93.0	93.5	90.5	96.0	102.9	81.5	85.8
AlSb	B3	58.2	64.6	65.9	71.2	72.5	69.5	74.2	79.3	59.2	63.7
GaN	B3	213.7	204.1	212.3	220.6	199.2	197.5	219.9	243.1	177.6	197.4
GaP	B3	92.3	94.0	96.6	104.1	106.2	101.2	107.8	116.7	87.2	90.2
GaAs	B3	78.0	77.6	79.7	88.3	88.0	84.3	92.3	101.1	66.9	75.2
GaSb	B3	57.9	56.1	56.6	71.1	71.6	66.9	54.3	52.9	53.1	60.5
InP	B3	72.0	75.5	77.3	84.8	87.4	81.9	89.0	96.3	71.3	74.8
InAs	B3	58.6	64.0	65.3	73.7	74.9	70.6	77.9	85.2	52.4	62.8
InSb	B3	46.1	51.8	52.4	60.9	62.6	58.1	64.0	70.1	40.2	51.2
ZnS	B3	75.0	82.7	81.7	86.6	84.1	83.2	88.4	95.2	76.9	85.4
ZnSe	B3	65.9	70.4	68.8	74.3	71.6	69.1	76.8	82.4	61.6	68.6
ZnTe	B3	52.8	54.3	52.6	58.4	56.2	53.4	60.7	65.0	43.4	51.7
CdTe	B3	45.0	45.1	43.6	48.6	48.2	45.3	50.7	55.1	36.3	45.2
MgS	B1	78.9	64.0	64.8	65.3	66.8	64.4	67.1	70.6	67.5	63.7
LiF	B1	76.3	81.1	79.3	74.8	74.0	69.5	74.9	83.3	69.2	73.6
LiCl	B1	38.2	37.4	36.1	32.6	38.5	33.1	36.8	39.9	35.6	30.7
NaF	B1	53.1	57.4	55.6	54.5	67.2	59.5	53.5	58.5	54.8	45.9
NaCl	B1	27.6	27.8	27.0	25.3	32.0	29.4	27.0	29.7	27.2	29.8
MgO	B1	169.8	178.5	182.9	177.7	167.6	170.4	179.6	193.2	176.4	150.7
SrTiO3	E21	179.0	207.4	209.1	206.3	190.0	192.0	205.9	229.9	183.9	206.2

Table 5: Reference data for band gaps (eV).

System	Symmetry	Exp.	HF	LDA	PBE	PBEsol	B97	B3LYP	PBE0	PBEsol0	HSE06
C	A4	5.49	12.37	4.20	4.14	4.05	5.74	5.91	6.00	5.94	5.35
Si	A4	1.17	6.26	0.55	0.72	0.58	1.75	1.84	1.82	1.72	1.25
Ge	A4	0.74	5.53	0.01	0.00	0.01	0.37	0.00	1.05	1.24	0.64
SiC	B3	2.42	8.51	1.38	1.46	1.32	2.80	3.00	2.94	2.85	2.30
BN	B3	6.36	13.60	4.42	4.49	4.32	6.36	6.51	6.53	6.42	5.84
BP	B3	2.40	7.79	1.31	1.39	1.27	2.63	2.76	2.73	2.65	2.10
BAs	B3	1.46	7.17	1.13	1.24	1.12	2.38	2.46	2.47	2.38	1.88
AlP	B3	2.49	8.07	1.57	1.84	1.63	3.10	3.18	3.16	3.01	2.51
AlAs	B3	2.23	7.78	2.24	1.75	1.56	2.95	3.01	3.01	2.87	2.38
AlSb	B3	1.69	6.73	1.20	1.31	1.25	2.36	2.23	2.50	2.40	1.92
GaN	B3	3.30	10.39	1.92	1.55	1.70	3.24	3.11	3.62	3.73	2.99
GaP	B3	2.35	7.65	1.57	1.67	1.66	2.83	2.53	3.08	2.91	2.46
GaAs	B3	1.52	6.61	0.43	0.19	0.42	1.25	0.82	1.73	1.87	1.27
GaSb	B3	0.81	5.73	0.09	0.00	0.06	0.68	0.28	1.22	1.39	0.79
InP	B3	1.42	7.04	0.81	0.67	0.82	1.72	1.38	2.18	2.25	1.66
InAs	B3	0.41	5.59	0.00	0.00	0.00	0.45	0.00	0.86	0.94	0.45
InSb	B3	0.23	5.21	0.00	0.00	0.00	0.28	0.00	0.75	0.88	0.35
ZnS	B3	3.84	9.75	2.20	2.12	2.18	3.60	3.38	4.00	4.02	3.39
ZnSe	B3	2.82	8.41	1.21	1.18	1.24	2.58	2.25	2.91	2.93	2.35
ZnTe	B3	2.39	7.93	1.27	1.12	1.26	2.36	2.01	2.77	2.86	2.22
CdTe	B3	1.61	6.85	0.61	0.62	0.67	1.69	1.42	2.03	2.04	1.57
MgS	B1	5.40	11.33	3.85	3.90	3.85	5.48	5.35	5.89	5.75	5.11
LiF	B1	14.20	22.46	9.97	9.26	9.44	12.05	12.04	12.67	12.83	11.89
LiCl	B1	9.40	15.06	6.75	6.48	6.55	8.31	8.17	8.75	8.79	8.00
NaF	B1	11.50	21.22	8.51	8.60	8.59	11.23	11.02	11.74	11.73	10.96
NaCl	B1	8.97	14.56	5.57	5.73	5.67	7.58	7.37	7.95	7.89	7.20
MgO	B1	7.80	15.79	5.05	4.45	4.61	6.74	6.80	7.20	7.37	6.51
SrTiO3	E21	3.25	11.76	1.73	1.72	1.73	3.46	3.35	3.82	3.95	3.96

Table 6: Reference data for band gaps (eV), continued.

System	Symmetry	Exp.	HSEsol	HISS	RSHXLDA	wB97	wB97X	LC-wPBE	LC-wPBEsol	M06-L	M06
C	A4	5.49	5.29	6.05	10.93	10.66	10.29	10.52	11.56	4.73	6.42
Si	A4	1.17	1.16	1.50	5.52	5.48	5.21	5.14	5.63	1.08	2.12
Ge	A4	0.74	0.76	1.12	4.56	4.67	4.10	4.74	5.27	0.16	0.47
SiC	B3	2.42	2.21	2.73	7.35	7.45	6.98	6.87	7.67	1.66	3.08
BN	B3	6.36	5.73	6.64	11.42	11.45	11.01	11.00	12.19	4.90	6.74
BP	B3	2.40	2.02	2.44	6.87	6.77	6.47	6.47	7.10	1.79	3.08
BAs	B3	1.46	1.79	2.15	6.36	6.31	6.01	6.00	6.55	1.52	2.57
AlP	B3	2.49	2.36	2.78	7.23	7.25	6.91	6.83	7.34	2.18	3.16
AlAs	B3	2.23	2.24	2.63	6.87	6.82	6.56	6.49	6.99	2.11	3.02
AlSb	B3	1.69	1.81	2.12	6.14	5.89	5.67	5.79	6.21	1.52	2.25
GaN	B3	3.30	3.09	4.06	8.80	8.17	7.69	8.40	10.00	1.90	3.72
GaP	B3	2.35	2.30	2.70	6.86	6.89	6.60	6.60	7.03	2.20	2.71
GaAs	B3	1.52	1.41	1.93	5.38	5.45	4.91	5.83	6.49	0.90	1.39
GaSb	B3	0.81	0.96	1.37	4.66	4.72	4.22	5.08	5.63	0.30	0.85
InP	B3	1.42	1.73	2.27	6.10	6.41	5.71	6.49	6.99	1.46	1.76
InAs	B3	0.41	0.53	0.99	4.23	4.36	3.89	4.81	5.58	0.17	0.64
InSb	B3	0.23	0.48	0.85	4.03	4.14	3.68	4.65	5.39	0.00	0.48
ZnS	B3	3.84	3.42	4.14	8.34	8.27	7.74	8.38	9.42	2.81	3.67
ZnSe	B3	2.82	2.37	3.00	6.81	6.74	6.38	7.00	7.95	1.83	2.74
ZnTe	B3	2.39	2.31	2.81	6.50	6.38	6.02	6.88	7.60	1.49	2.39
CdTe	B3	1.61	1.59	2.05	5.58	5.29	4.98	5.87	6.51	0.94	1.65
MgS	B1	5.40	5.06	5.68	10.33	10.05	9.80	10.03	10.64	4.63	5.73
LiF	B1	14.20	12.05	13.41	18.10	17.28	16.91	17.71	20.11	10.23	12.46
LiCl	B1	9.40	8.04	8.93	13.68	13.43	12.82	13.68	14.92	7.50	8.55
NaF	B1	11.50	10.96	12.38	16.98	16.52	16.19	17.00	18.94	10.10	11.83
NaCl	B1	8.97	7.15	8.10	12.79	12.56	12.13	12.89	13.98	7.24	8.15
MgO	B1	7.80	6.68	7.94	12.67	11.92	11.49	12.09	14.31	5.23	7.29
SrTiO3	E21	3.25	3.16	3.96	8.24	7.98	7.69	8.28	9.64	2.47	4.12

Table 7: Validation data for lattice constants (Å).

System	Symmetry	Exp.	HF	LDA	PBE	PBEsol	B97	B3LYP	PBE0	PBEsol0	HSE06
AlN	B3	4.368	4.371	4.349	4.408	4.382	4.391	4.396	4.371	4.354	4.373
CdS	B3	5.808	6.043	5.767	5.948	5.844	5.961	5.986	5.898	5.830	5.903
CdSe	B3	6.042	6.299	6.021	6.207	6.094	6.217	6.249	6.148	6.072	6.154
MgSe	B1	5.375	5.566	5.397	5.512	5.455	5.519	5.529	5.470	5.432	5.474
MgTe	B1	6.410	6.572	6.356	6.495	6.428	6.497	6.517	6.453	6.404	6.458
BaS	B1	6.364	6.608	6.300	6.438	6.352	6.479	6.504	6.414	6.355	6.417
BaSe	B1	6.570	6.866	6.515	6.673	6.576	6.713	6.745	6.650	6.583	6.654
BaTe	B1	6.982	7.324	6.892	7.069	6.959	7.119	7.163	7.051	6.976	7.055
LiH	B1	3.979	4.109	3.905	4.004	3.976	4.019	4.004	3.989	3.970	3.989

Table 8: Validation data for lattice constants (Å), continued.

System	Symmetry	Exp.	HSEsol	HISS	RSHXLDA	wB97	wB97X	LC-wPBE	LC-wPBEsol	M06-L	M06
AlN	B3	4.368	4.355	4.351	4.350	4.392	4.381	4.358	4.322	4.349	4.359
CdS	B3	5.808	5.833	5.866	5.830	5.865	5.892	5.819	5.768	5.944	5.897
CdSe	B3	6.042	6.078	6.113	6.063	6.127	6.147	6.051	5.997	6.243	6.154
MgSe	B1	5.375	5.435	5.452	5.428	5.508	5.507	5.414	5.384	5.492	5.509
MgTe	B1	6.410	6.408	6.433	6.398	6.462	6.473	6.380	6.344	6.487	6.466
BaS	B1	6.364	6.358	6.400	6.463	6.435	6.454	6.390	6.364	6.418	6.412
BaSe	B1	6.570	6.586	6.638	6.694	6.708	6.712	6.621	6.591	6.701	6.652
BaTe	B1	6.982	6.978	7.041	7.105	7.114	7.124	7.017	6.991	7.116	7.083
LiH	B1	3.979	3.968	3.977	4.143	4.084	4.101	3.988	3.972	4.030	4.138

Table 9: Validation data for band gaps (eV).

System	Symmetry	Exp.	HF	LDA	PBE	PBEsol	B97	B3LYP	PBE0	PBEsol0	HSE06
AlN	B3	5.34	12.14	3.37	3.45	3.31	5.22	5.35	5.39	5.30	4.70
CdS	B3	2.58	8.26	1.02	1.10	1.08	2.46	2.24	2.79	2.72	2.17
CdSe	B3	1.85	7.12	0.34	0.48	0.45	1.68	1.42	1.97	1.91	1.45
MgSe	B1	2.47	8.59	1.64	1.71	1.71	3.07	2.98	3.33	3.32	2.62
MgTe	B1	3.60	9.60	3.01	2.92	2.99	4.24	4.06	4.54	4.59	3.98
BaS	B1	3.88	9.29	1.99	2.39	2.15	3.80	3.75	3.95	3.75	3.26
BaSe	B1	3.58	8.67	1.69	2.05	1.83	3.42	3.36	3.51	3.33	2.85
BaTe	B1	3.08	8.01	1.41	1.80	1.56	3.06	3.05	3.12	2.93	2.49
LiH	B1	4.94	11.02	2.62	3.10	2.84	4.78	4.85	4.76	4.57	4.10

Table 10: Validation data for band gaps (eV), continued.

System	Symmetry	Exp.	HSEsol	HISS	RSHXLDA	wB97	wB97X	LC-wPBE	LC-wPBEsol	M06-L	M06
AlN	B3	5.34	4.61	5.41	10.24	10.28	9.80	9.72	10.90	3.77	5.80
CdS	B3	2.58	2.13	2.78	6.99	6.78	6.34	7.11	7.85	1.63	2.43
CdSe	B3	1.85	1.41	1.98	5.71	5.75	4.96	5.93	6.77	0.98	1.74
MgSe	B1	2.47	2.62	3.09	7.49	7.56	7.21	7.46	8.22	2.48	3.51
MgTe	B1	3.60	4.03	4.56	8.53	8.34	7.98	8.55	9.30	3.78	4.71
BaS	B1	3.88	3.08	3.66	8.21	7.92	7.68	8.07	8.55	2.61	3.71
BaSe	B1	3.58	2.68	3.18	7.62	7.34	7.15	7.42	7.87	2.26	3.45
BaTe	B1	3.08	2.30	2.75	7.10	6.76	6.60	6.83	7.19	1.88	2.95
LiH	B1	4.94	3.90	4.67	9.30	9.51	9.16	8.86	9.71	4.09	5.83

Table 11: Calibration and prediction uncertainty parameters for lattice constants (Å).

	a	b	d^2	$u^2(a)$	$u^2(b)$	$u(a,b)$
HF	0.265844	0.930312	0.002249	0.002848	0.000098	-0.000522
LDA	0.030841	1.000760	0.000744	0.001030	0.000038	-0.000194
PBE	0.092315	0.965792	0.000557	0.000754	0.000026	-0.000139
PBEsol	0.017136	0.992155	0.000222	0.000310	0.000011	-0.000058
B97	0.115161	0.961603	0.000553	0.000742	0.000026	-0.000137
B3LYP	0.177782	0.947511	0.000573	0.000750	0.000026	-0.000138
PBE0	0.081523	0.977020	0.000343	0.000466	0.000017	-0.000087
PBEsol0	0.054438	0.990608	0.000285	0.000392	0.000014	-0.000074
HSE06	0.090796	0.974474	0.000329	0.000446	0.000016	-0.000083
HSEsol	0.046161	0.991261	0.000166	0.000230	0.000008	-0.000043
HISS	0.063423	0.985647	0.000441	0.000603	0.000022	-0.000113
RSHXLDA	-0.033043	1.008890	0.001498	0.002125	0.000077	-0.000399
wB97	-0.045111	1.003750	0.000753	0.001073	0.000038	-0.000200
wB97X	0.014397	0.989527	0.000989	0.001378	0.000049	-0.000256
LC-wPBE	-0.087521	1.020460	0.001154	0.001670	0.000061	-0.000314
LC-wPBEsol	-0.068626	1.025370	0.001005	0.001444	0.000053	-0.000274
M06-L	0.225104	0.944739	0.001756	0.002258	0.000079	-0.000417
M06	0.101464	0.969896	0.001686	0.002274	0.000080	-0.000421

Table 12: Calibration and prediction uncertainty parameters for bulk modulus (GPa).

	a	b	d^2	$u^2(a)$	$u^2(b)$	$u(a,b)$
HF	5.299730	0.907086	60.9892	5.14927	0.000184	-0.022823
LDA	-2.879920	0.991786	69.1134	6.27555	0.000248	-0.030138
PBE	5.744720	1.056710	70.3462	5.86778	0.000286	-0.030320
PBEsol	1.259210	1.025550	61.0518	5.36143	0.000236	-0.026757
B97	4.004020	1.026530	56.3024	4.83764	0.000219	-0.024232
B3LYP	6.673300	1.023960	64.8168	5.38080	0.000249	-0.026957
PBE0	2.248060	0.976575	48.8665	4.31274	0.000173	-0.020508
PBEsol0	-0.829878	0.959953	50.2026	4.55636	0.000172	-0.021222
HSE06	2.902020	0.978135	49.6329	4.34764	0.000177	-0.020722
HSEsol	0.188090	0.959255	51.0952	4.58604	0.000174	-0.021372
HISS	2.367750	0.920349	44.2389	3.92973	0.000141	-0.017610
RSHXLDA	-4.090890	0.948504	59.9397	5.55014	0.000198	-0.025438
wB97	-10.665400	1.025490	87.1653	8.44242	0.000331	-0.041432
wB97X	-5.779100	1.009880	70.1773	6.54815	0.000261	-0.031886
LC-wPBE	-5.247850	0.940126	78.2386	7.22576	0.000251	-0.032792
LC-wPBEsol	-5.817900	0.878467	88.9413	8.21588	0.000248	-0.034823
M06-L	3.655850	1.006760	84.4851	7.13272	0.000310	-0.035067
M06	0.290985	1.005680	92.5850	8.04863	0.000337	-0.039392

Table 13: Calibration and prediction uncertainty parameters for band gaps (eV).

	a	b	d^2	$u^2(a)$	$u^2(b)$	$u(a,b)$
HF	-3.772960	0.769666	0.491559	0.104197	0.000884	-0.008753
LDA	0.500446	1.346620	0.217512	0.015008	0.001173	-0.002913
PBE	0.502391	1.384660	0.322265	0.022307	0.001852	-0.004471
PBEsol	0.503246	1.385130	0.209227	0.014420	0.001193	-0.002878
B97	-0.476155	1.141850	0.275901	0.025245	0.001074	-0.004066
B3LYP	-0.196524	1.107580	0.446166	0.037994	0.001656	-0.006044
PBE0	-0.818884	1.131900	0.163279	0.016354	0.000619	-0.002553
PBEsol0	-0.834921	1.133530	0.120907	0.012141	0.000459	-0.001894
HSE06	-0.292955	1.166900	0.189684	0.016416	0.000766	-0.002718
HSEsol	-0.268050	1.167400	0.114798	0.009836	0.000462	-0.001627
HISS	-0.593722	1.064800	0.136763	0.012853	0.000458	-0.001911
RSHXLDA	-4.051670	0.947657	0.268522	0.059576	0.000720	-0.005998
wB97	-4.328140	0.998028	0.292030	0.068768	0.000870	-0.007123
wB97X	-3.909350	0.995743	0.316932	0.068420	0.000941	-0.007332
LC-wPBE	-4.312070	0.986559	0.182869	0.042622	0.000528	-0.004364
LC-wPBEsol	-4.174930	0.871636	0.274368	0.062503	0.000622	-0.005727
M06-L	0.166347	1.240360	0.312359	0.023821	0.001439	-0.004269
M06	-0.567563	1.093080	0.319148	0.030024	0.001143	-0.004613