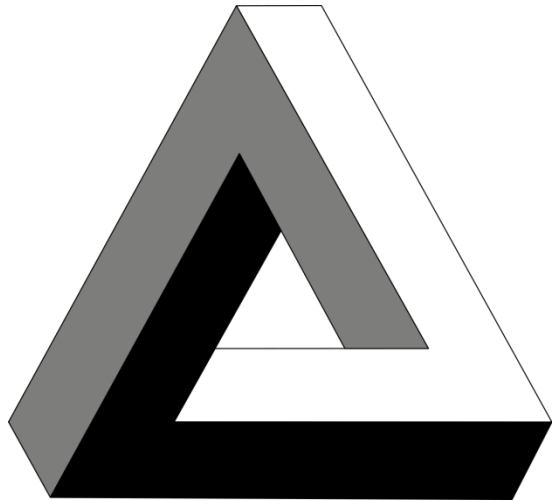


THE DELTA PROJECT: CURRENT STATUS AND FUTURE DIRECTIONS



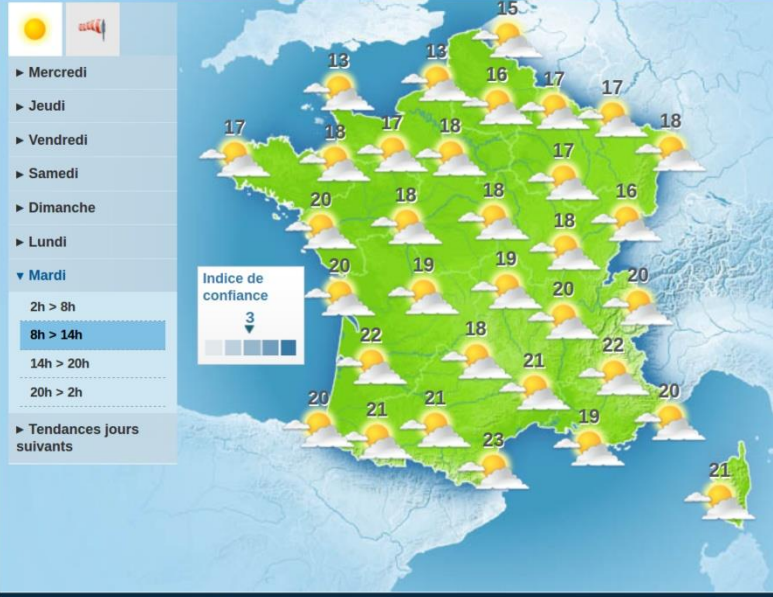
Kurt Lejaeghere

Center for Molecular Modeling
Ghent University, Belgium

together with

Stefaan Cottenier

the Delta collaboration



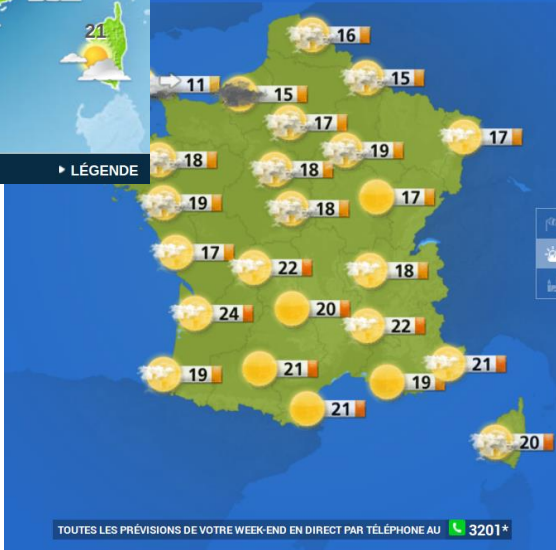




Prévisions météo actualisées à 12h29

► LÉGENDE

Les hautes pressions devraient garantir un temps sec et assez bien ensoleillé, avec le retour de la saison l'après-midi.



TOUTES LES PRÉVISIONS DE VOTRE WEEK-END EN DIRECT PAR TÉLÉPHONE AU 3201*



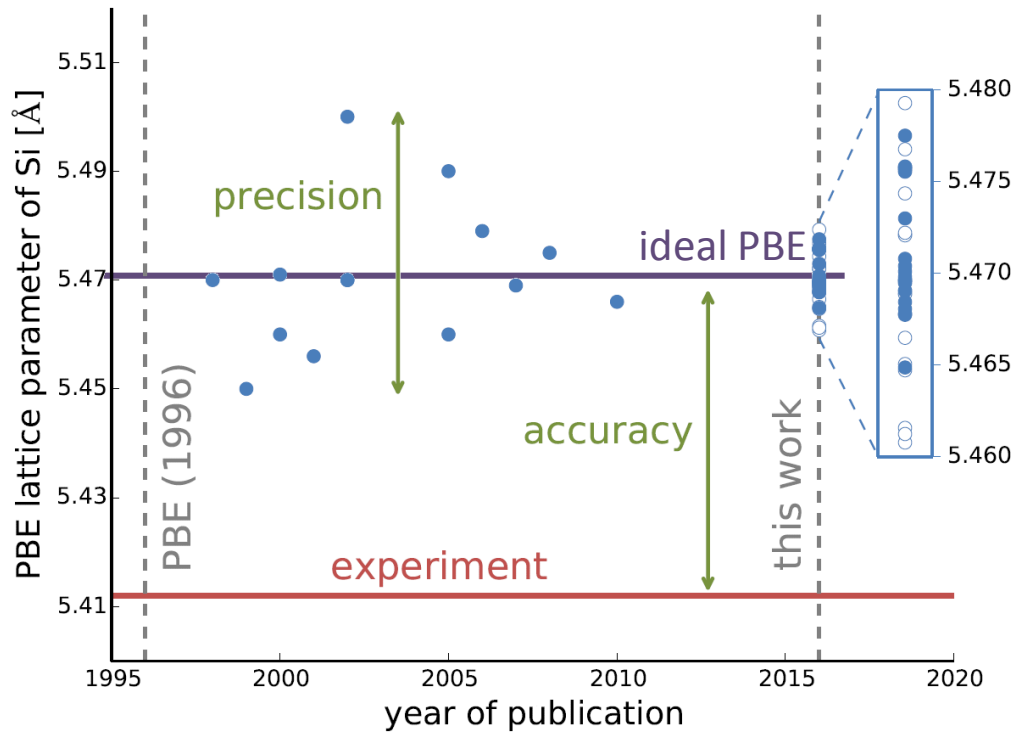


- Mercredi
- Jeudi
- Vendredi
- Samedi
- Dimanche
- Lundi
- ▼ **Mardi**
 - 2h > 8h
 - 8h > 14h**
 - 14h > 20h
 - 20h > 2h
- Tendances jours suivants

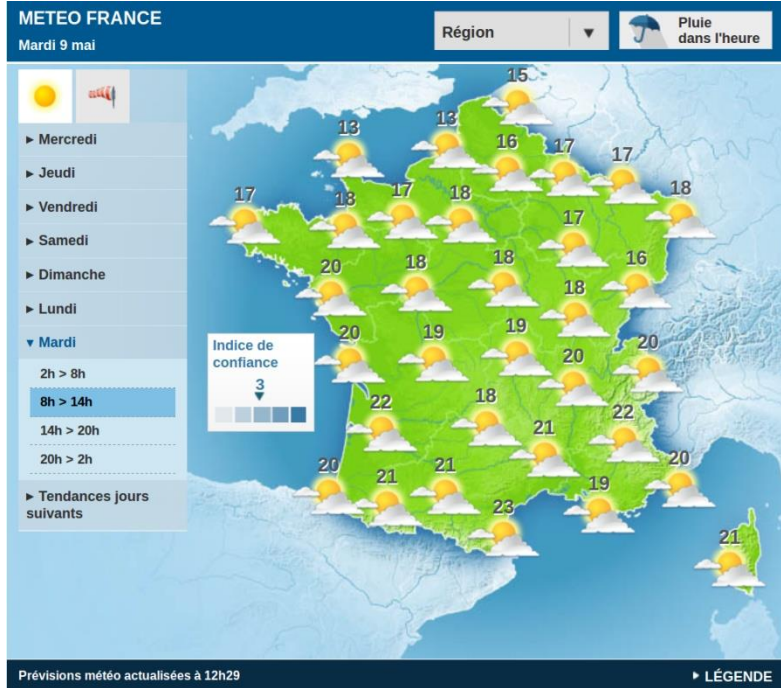
Les hautes pressions devraient garantir un temps sec et assez bien ensoleillé, avec le retour de la saison l'après-midi.



- MER 3
- JEU 4
- VEN 5
- SAM 6**
- DIM 7
- LUN 8
- MAR 9**
- MATIN
- APRÈS-MIDI
- SOIR
- NUIT
- MER 10
- JEU 11
- VEN 12
- SAM 13
- DIM 14
- LUN 15
- MAR 16
- MER 17

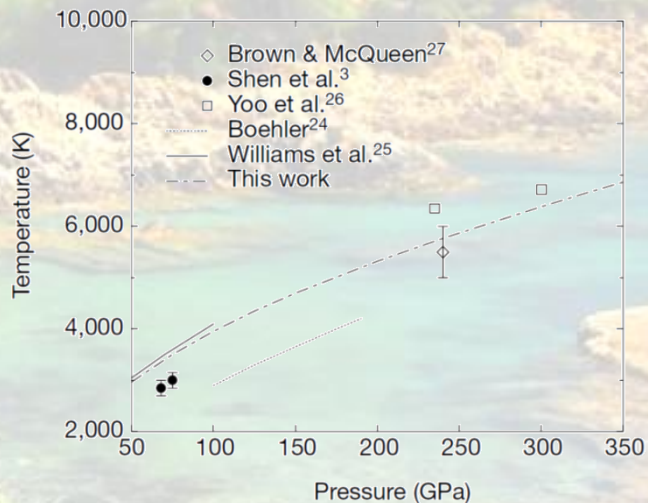
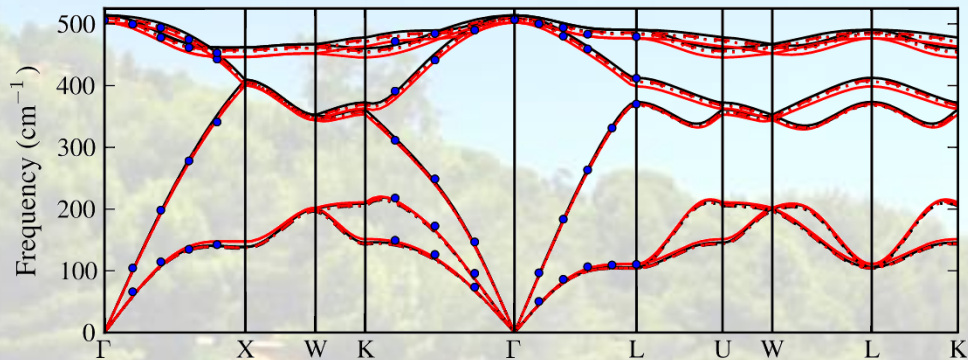


KL and 68 others, Science 351 (6280), aad3000 (2016).



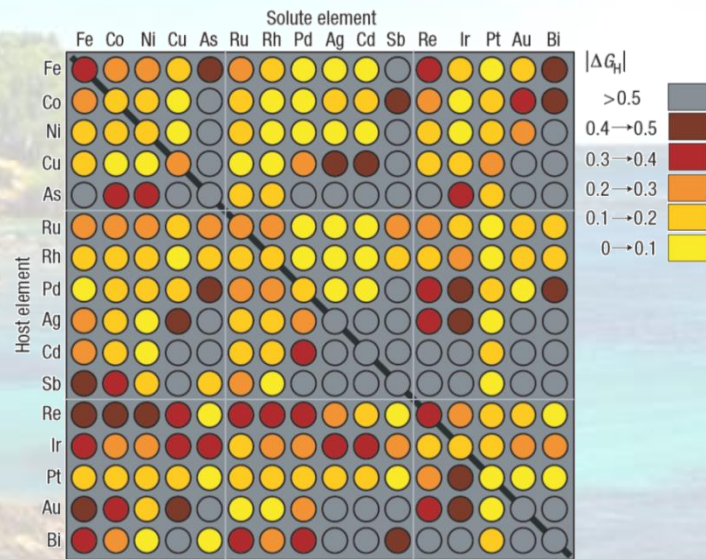
ACCURACY

He et al., PRB 89, 064305 (2014)

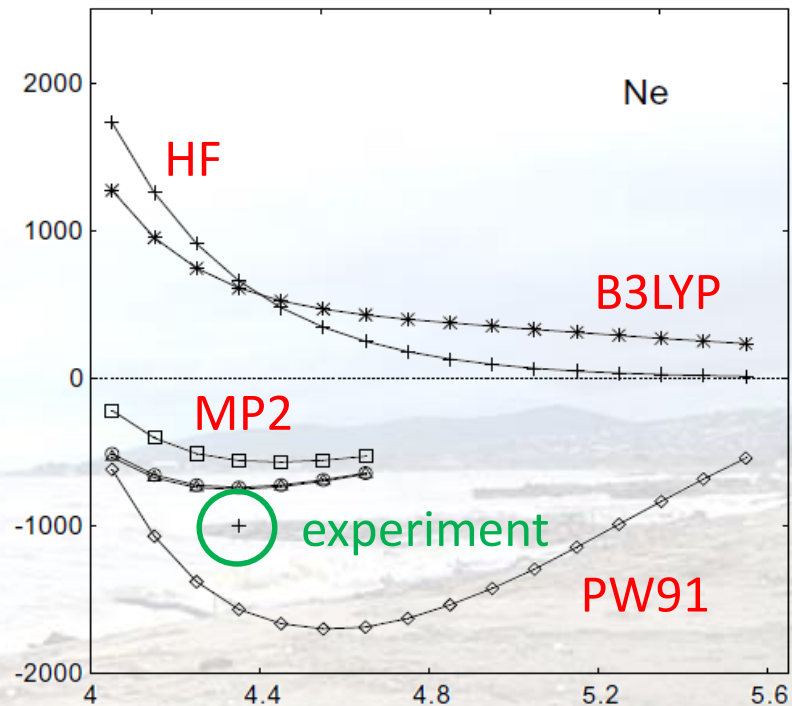
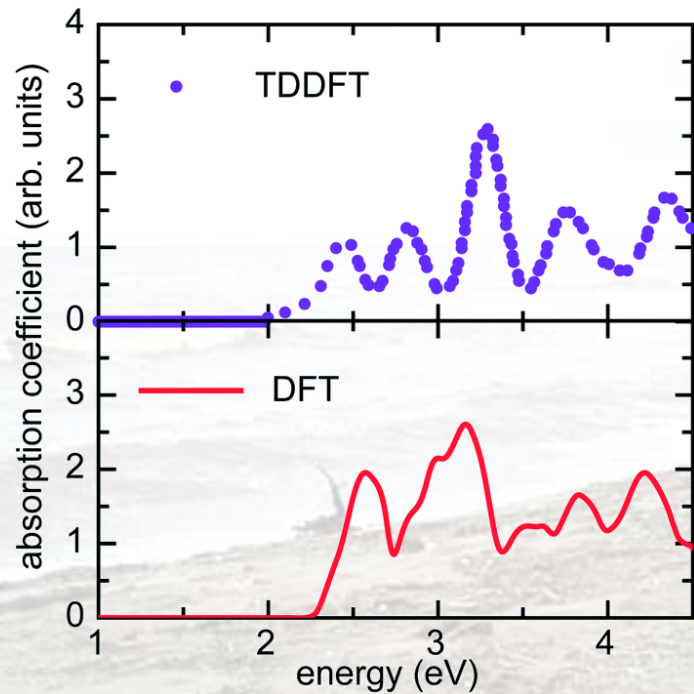


Alfè et al., Nature 401, 462 (1999)

Greeley et al., Nature Mater. 5, 909 (2006)



Hidalgo et al., *Nanoscale* 6, 3325
(2014)



Halo et al., *Chem. Phys. Lett.* 467, 294
(2009)



Tran, Stelzl, and Blaha

J. Chem. Phys. **144**, 204120 (2016)

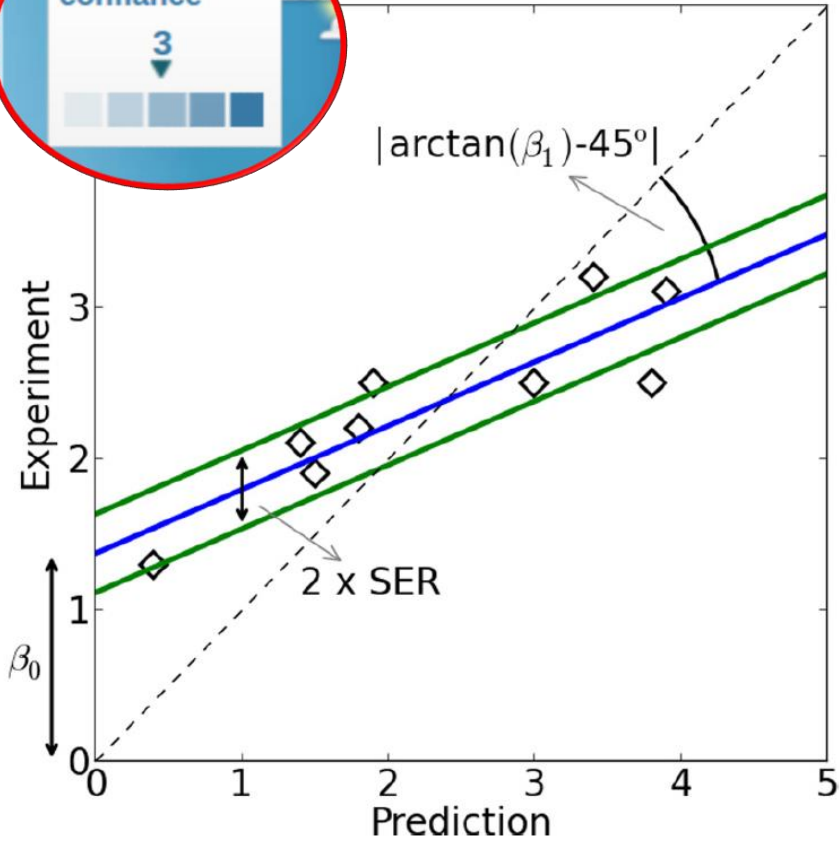
not reflect the trends for finite systems, as mentioned in Sec. III. Thus, in order to provide to the reader of the present work a more general view on the accuracy and applicability of the functionals, a very brief summary of some of the literature results for molecular systems is given below. To this end, we consider the atomization energy of strongly bound molecules and the interaction energy between weakly bound molecules, for which widely used standard testing sets exist.

A. Atomization energy of molecules

The atomization energy of molecules is one of the most

TABLE V. Results from the literature (reference in last column) for the MAE (in kcal/mol) on the S22 testing set.

Functional	MAE	Reference
LDA		
LDA ⁸⁰	2.3	48
GGA		
PBEsol ⁸³	1.8	48
PBE ⁷³	2.8	48
RPBE ⁹²	5.2	49
revPBE ⁹¹	5.3	27
BLYP ^{93,94}	4.8, 8.8	106, 48



$$Y = \beta_0 + \beta_1 X \pm \text{SER}$$



$\beta_0 ; \beta_1 - 1$
systematic
deviation

SER
error bar



functional error



Prévisions météo actualisées à 12h29

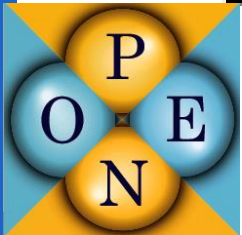
LÉGENDE

Les hautes pressions devraient garantir un temps sec et assez bien ensoleillé, avec le retour de la saison l'après-midi.



PRECISION

AIMPRO.abinit



GPAW!

CASTEP **leur**



ADF

b-initio

siesta

binit

RSP

VAPO-CHEM

QUANTUMESPRESSO

**Atomistix
ToolKit**

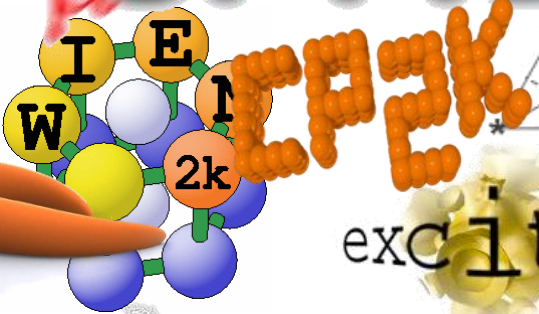


A QUANTUM LEAP INTO THE FUTURE

TUB BON OLE GmbH



siesta

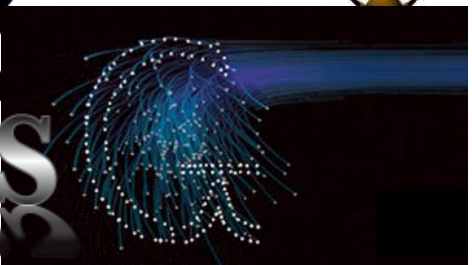
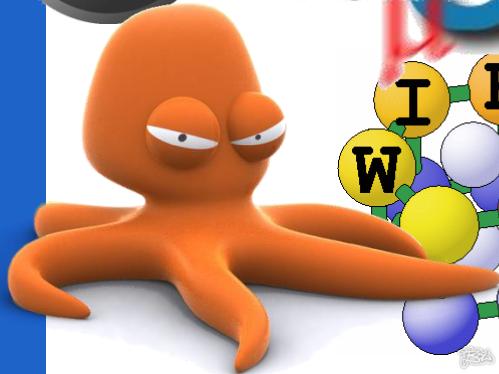


a computational tool for solid state chemistry and physics



Qbox
First-Princi

exciting **GAMES**



RESEARCH ARTICLE

DFT METHODS

Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere,^{1*} Gustav Bihlmayer,² Torbjörn Björkman,^{3,4} Peter Blaha,⁵ Stefan Blügel,² Volker Blum,⁶ Damien Caliste,^{7,8} Ivano E. Castelli,⁹ Stewart J. Clark,¹⁰ Andrea Dal Corso,¹¹ Stefano de Gironcoli,¹¹ Thierry Deutsch,^{7,8} John Kay Dewhurst,¹² Igor Di Marco,¹³ Claudia Draxl,^{14,15} Marcin Dułak,¹⁶ Olle Eriksson,¹³ José A. Flores-Livas,¹² Kevin F. Garrity,¹⁷ Luigi Genovese,^{7,8} Paolo Giannozzi,¹⁸ Matteo Giantomassi,¹⁹ Stefan Goedecker,²⁰ Xavier Gonze,¹⁹ Oscar Grånäs,^{13,21} E. K. U. Gross,¹² Andris Gulans,^{14,15} François Gygi,²² D. R. Hamann,^{23,24} Phil J. Hasnip,²⁵ N. A. W. Holzwarth,²⁶ Diana Iușan,¹³ Dominik B. Jochym,²⁷ François Jollet,²⁸ Daniel Jones,²⁹ Georg Kresse,³⁰ Klaus Koepfner,^{31,32} Emine Küçükbenli,^{9,11} Yaroslav O. Kvashnin,¹³ Inka L. M. Locht,^{13,33} Sven Lubeck,¹⁴ Martijn Marsman,³⁰ Nicola Marzari,⁹ Ulrike Nitzsche,³¹ Lars Nordström,¹³ Taisuke Ozaki,³⁴ Lorenzo Paulatto,³⁵ Chris J. Pickard,³⁶ Ward Poelmans,^{1,37} Matt I. J. Probert,²⁵ Keith Refson,^{38,39} Manuel Richter,^{31,32} Gian-Marco Rignanese,¹⁹ Santanu Saha,²⁰ Matthias Scheffler,^{15,40} Martin Schlipf,²² Karlheinz Schwarz,⁵ Sangeeta Sharma,¹² Francesca Tavazza,¹⁷ Patrik Thunström,⁴¹ Alexandre Tkatchenko,^{15,42} Marc Torrent,²⁸ David Vanderbilt,²³ Michiel J. van Setten,¹⁹ Veronique Van Speybroeck,¹ John M. Wills,⁴³ Jonathan R. Yates,²⁹ Guo-Xu Zhang,⁴⁴ Stefaan Cottenier^{1,45*}

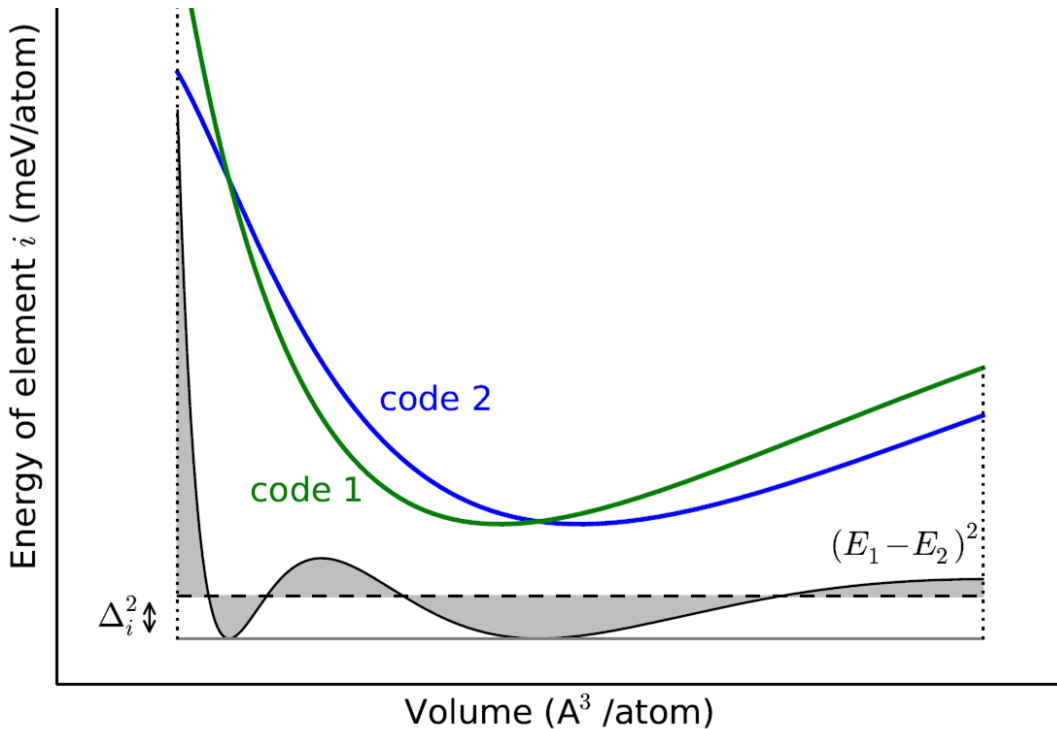
The widespread popularity of density functional theory has given rise to an extensive range

of the fundamental variable. Although this reformulation is in principle exact, it is not fully known how the interaction between individual electrons should be transformed. As a result, the specific form of the unknown part of the interaction energy, the exchange-correlation functional, has been the focus of many investigations, leading to a plethora of available functionals in both solid-state physics (15–19) and quantum chemistry (15, 20–23).

Once a particular exchange-correlation functional has been chosen, the mathematical problem is completely specified as a set of Kohn-Sham equations, whose solution yields orbitals and energies from which the total electronic energy can be evaluated. A variety of such numerical solution schemes have been implemented in different computer codes. Comparisons of their performance are much less frequent or extensive than those of exchange-correlation functionals, however (21, 24–29). One might reasonably expect that because they solve the same equations, they all produce similar answers for a given crystal structure, but a glance at the literature shows that this assumption is by no means always true. Figure 1 demonstrates that even for a well-studied material such as silicon, deviations between predictions from different codes (the “precision”) are of the same order of magnitude as the deviation from the 0 K experimental value (the “accuracy”) (26, 30). Because all of the codes shown in Fig. 1 treat silicon at the same level of theory, using the same exchange-correlation functional, they yield the same accuracy by definition. However

H																		He
194																		194
hP4																		hP2
Li	Be											B	C	N	O	F		Ne
166	194											166	194	205	12	15		225
hR9	hP2											hR36	hP4	cP8	mS4	mS8		cF4
Na	Mg											Al	Si	P	S	Cl		Ar
166	194											225	227	64	70	64		225
hR9	hP2											cF4	cF8	oS8	oF128	oS8		cF4
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br		Kr
229	225	194	194	229	229	217	229	194	225	225	194	64	227	166	152	64		225
cI2	cF4	hP2	hP2	cI2	cI2	cI58	cI2	hP2	cF4	cF4	hP2	oS8	cF8	hR6	hP3	oS8		cF4
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I		Xe
229	225	194	194	229	229	194	194	225	225	225	194	139	227	166	152	64		225
cI2	cF4	hP2	hP2	cI2	cI2	hP2	hP2	cF4	cF4	cF4	hP2	tI2	cF8	hR6	hP3	oS8		cF4
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At		Rn
229	229	194	194	229	229	194	194	225	225	225	139	194	225	166	221			225
cI2	cI2	hP2	hP2	cI2	cI2	hP2	hP2	cF4	cF4	cF4	tI2	hP2	cF4	hR6	cP1			cF4

- large number of elements
- diverse set of crystal structures



$$\Delta_i(1, 2) = \sqrt{\frac{1}{\Delta V_i} \int (E_{1,i}(V) - E_{2,i}(V))^2 dV}$$

$$\Delta(1, 2) = \langle \Delta_i(1, 2) \rangle$$



molmod.ugent.be/deltacodesdft

	version			meV/atom
VASP	5.2.12	plane waves	PAW 2015 GW-ready (5.4)	0.3 meV/atom
FHI-aims	081213	tier2 numerical orbitals	all-electron (relativistic zora scalar 1e-12)	0.3 meV/atom
Quantum ESPRESSO	5.1	plane waves	SSSP Accuracy (mixed NC/US/PAW potential library)	0.3 meV/atom
Elk	3.1.5	APW+lo	all-electron	0.3 meV/atom
ABINIT	7.8.2	plane waves	PAW JTH v1.0	0.4 meV/atom
FLEUR	0.26	LAPW (+lo)	all-electron	0.4 meV/atom
Quantum ESPRESSO	5.1	plane waves	SSSP Efficiency (mixed NC/US/PAW potential library)	0.4 meV/atom
CASTEP	9.0	plane waves	OTFG CASTEP 9.0	0.5 meV/atom
ABINIT	7.7.3	plane waves	PAW JTH v0.2	0.5 meV/atom
FHI-aims	081213	tight numerical orbitals	all-electron (relativistic atomic_zora scalar)	0.5 meV/atom
VASP	5.2.12	plane waves	PAW 2012	0.6 meV/atom
ABINIT	7.11.8	plane waves	pseudo_dojo_ONCVSPSP 0.1 norm-conserving	0.6 meV/atom

what's next?

code X vs code Y			TEST SYSTEMS				
			<i>basic</i>	<i>intermediate</i>	<i>advanced 1</i>	<i>advanced 2</i>	...
			crystal class 1	crystal class 2	crystal class 3	[extendable]	...
PROPERTIES	<i>basic</i>	property 1a	1 number	1 number	1 number
		property 2a	1 number	1 number	1 number
		property 3a	1 number	1 number	1 number
	<i>intermediate</i>	property 1b	1 number	1 number	1 number
		property 2b	1 number	1 number	1 number
		property 3b	1 number	1 number	1 number
	<i>advanced 1</i>	property 1c	1 number	1 number	1 number
		property 2c	1 number	1 number	1 number
		[extendable]

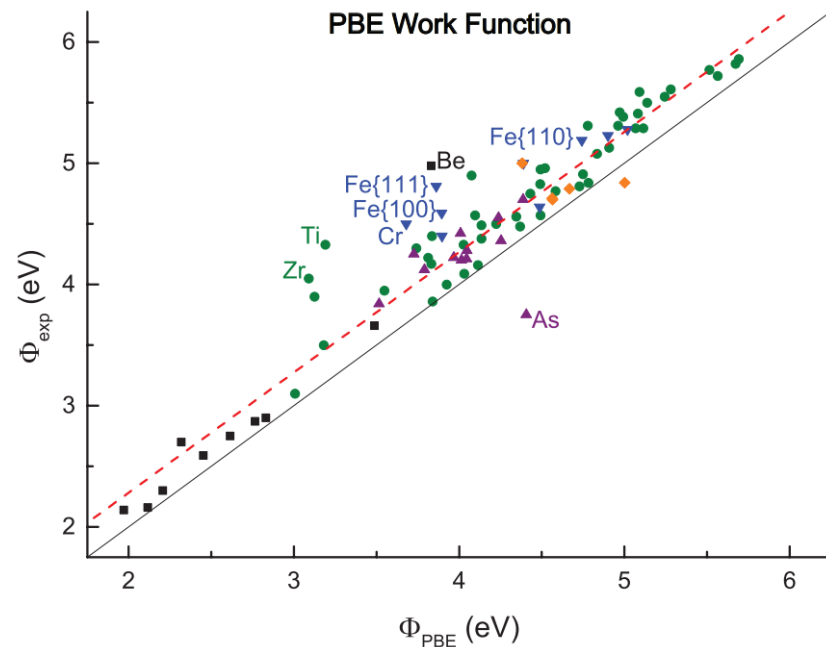
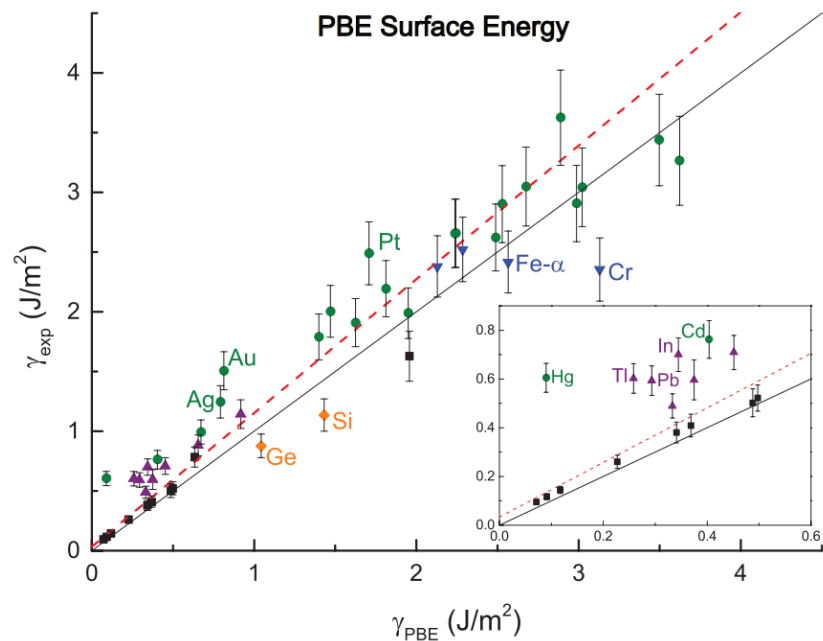
test systems

- structural diversity
all elemental crystals with fcc, bcc, sc and diamond structure (12/8/6/4 neighbours)
- chemical diversity
all oxides X_2O , XO , X_2O_3 , XO_2 , X_2O_5 and XO_3 (oxidation numbers +1 to +6)
- bond diversity (validation?)
for each element an experimentally known binary metal, ionic and covalent compound

properties

- formation energies
- band structures
- forces
- phonon frequencies
- magnetization
- ...

	β_0	$1 - \beta_1$	SER
Φ [eV]	0.30	1 %	1.29
γ [J/m ²]	0.03	-12 %	2.34



De Waele et al., PRB 94, 235418 (2016)

methodologies

- hybrid-functional DFT
- meta-GGA DFT
- GW
- BSE
- RPA
- ...



Reproducibility in density functional theory calculations of solids

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S. De Waele, W. Poelmans, A. Strobbe