J Mol Model (2013) 19:2791–2796
DOI 10.1007/s00894-012-1646-2

ORIGINAL PAPER

Assessing modern GGA functionals for solids

Frédéric Labat · Eric Brémond · Pietro Cortona · Carlo Adamo

Received: 28 August 2012 / Accepted: 11 October 2012 / Published online: 8 November 2012

Abstract We present periodic calculations carried out with Gaussian-type basis sets on a test set of 21 solids with nine exchange-correlation functionals, extending previous works performed with two parameter-free correlation functionals (TCA and revTCA) which showed promising results for molecules in terms of key structural and energetic properties. Two LDAs and seven GGAs were considered for the prediction of equilibrium lattice constants, bulk moduli, and cohesive energies, using the same test set for all properties when possible. The effect of combining the TCA correlation with exchange potentials other than the PBE form originally used is also addressed. We find that the previously noted good accuracy of the parameter-free TCA functional for molecules also holds for solids, as long as a modified form of the exchange potential that is more biased towards solids than PBE is taken into account. In particular, the PBEsolTCA functional performs well overall for the three key structural and energetic properties considered here.

Electronic supplementary material The online version of this article (doi:10.1007/s00894-012-1646-2) contains supplementary material, which is available to authorized users.

F. Labat (✉) · E. Brémond · C. Adamo
Laboratoire d'Électrochimie, Chimie des Interfaces et
Modélisation pour l'Énergie, UMR CNRS 7575,
ENSCP—Chimie Paristech,
11 rue P. et M. Curie,
Paris Cedex 05 75231, France
e-mail: frederic-labat@chimie-paristech.fr

P. Cortona
Laboratoire Structures, Propriétés et Modélisation des Solides
(SPMS), UMR CNRS 8580, École Centrale Paris,
Grande Voie des Vignes,
Châtenay-Malabry 92295, France

C. Adamo
Institut Universitaire de France,
103 Boulevard Saint Michel,
Paris 75005, France

Keywords DFT · Solids · Solid state · Periodic · PBC

Introduction

The Kohn–Sham (KS) approach to density functional theory [1] is a popular computational tool for many-electron systems, with a wide range of applications. In practice, an approximation to the exchange-correlation contribution is needed, and many such approximations have been proposed, ranging from the most simple to the most sophisticated forms occupying the five rungs of Jacob's ladder [2]. Although functionals of the fourth rung (hybrids based on the addition of a certain amount of Hartree–Fock (HF) nonlocal exact exchange to the KS exchange) are now well established for both molecular and nonmetallic solid-state calculations [3], they remain more computationally demanding than lower level approximations, such as those based on the generalized gradient approximation (GGA, second rung). This is particularly true when large or extended systems such as solids are considered, since the evaluation of the HF contribution to the exchange remains costly in this last case, especially in plane wave based codes. Since third-rung functionals (meta-GGA) such as TPSS [4], revTPSS [5], M06-L [6], or M11-L [7] have so far been shown to give results that are a little disappointing for solid-state calculations, several groups have recently proposed new GGA functionals [6, 8–18] in order to improve upon the performance of the standard Perdew–Burke–Ernzerhof (PBE) functional [19] routinely considered for solids.

When evaluating the performances of functionals, the total energy as well as its first and second derivatives with respect to various differentiating variables are commonly examined. In particular, for solids, the most popular calculations performed are probably those of equilibrium lattice constants (from the first derivative of the total energy with respect to the lattice basis vectors), the cohesive energy (from the total energy difference), and the bulk modulus (from the second derivative of the total energy with respect to the unit cell volume). Unfortunately, for most of the new GGA functionals mentioned above, the trends are similar for both solids and molecules: structural properties are generally more accurate than those given by PBE, but the cost of this extra accuracy is degradation of the cohesive or atomization energy predictions [5, 13, 14, 20–23].

Two notable exceptions are the very recently introduced functionals HTBS [13] and N12 [15], both of which are parametrized to perform well in terms of energetics and structures.

In a different spirit, we recently proposed two new parameter-free GGA correlation functionals, TCA and revTCA (see "Computational details" for details), which show good accuracy for molecules, significantly improving upon PBE for atomization energies (even yielding data close to that obtained with global hybrid functionals [24–26]), and providing structural data at least as good as that of PBE. In this contribution, we extend this work and assess the performances of these parameter-free correlation functionals for solids, considering equilibrium lattice constants, bulk moduli, and cohesive energy determination, using the same test set for all properties when possible. The effect of combining the TCA correlation with exchange potentials other than the PBE form originally used is also addressed.

We first provide computational details of our work, before presenting and discussing our results, and finally drawing some conclusions based on them.

Computational details

All calculations were carried out with a locally modified development version of Gaussian [27], using the available periodic boundary conditions code [28] based on localized (Gaussian-type orbital, GTO) basis sets. In order to provide a straightforward comparison with previously published works, the basis sets chosen were those previously refered to as GTO2, which were described and used in [12, 29, 30] and shown to provide data in line with more popular projector-augmented wave (PAW) results.

The chosen bulk systems test set is similar to that previously considered by Heyd et al. [31] and Paier et al. [32]; that is, the normal nonmagnetic structures of 21 solids [4] belonging to four families of crystalline systems: three metals (Li, Na, Al), nine semiconductors (BN, BP, C, Si, SiC, Ge, β-GaN, GaP, GaAs), five ionic solids (LiF, LiCl, NaF, NaCl, MgO), and four transition metals (Cu, Rh, Pd, Ag). **k**-point meshes with at least 16 points in each direction were found to be sufficient to converge the presented data to within specified digits.

In this work, we considered nine exchange-correlation functionals: (i) SVWN5 [33, 34], mainly used as an LDA reference; (ii) PBE [19], a GGA routinely used for solids; (iii) PBEsol [12], developed with solids in mind, and having the same analytical form as PBE in the exchange but with two modified parameters and an additional physical constraint in the correlation; (iv) SOGGA [6], built with an analytical form of the exchange enhancement factor that is an average of the PBE and RPBE ones [35], and which (like PBEsol) has already been shown to clearly improve on the original PBE for lattice constants but perform much worse than it for cohesive energies [6, 15, 30]. We also performed calculations with: (v) the original local correlation of Ragot and Cortona [36] combined with the Slater exchange [33] (SRC04 in the following), and subsequent modifications including gradient corrections: (vi) TCA [24] combined with the PBE exchange (TCA in the following), which satisfies two more physical constraints than the original RC04 functional, and (vii) revTCA [25] combined with a modified version of the PBE exchange [25] (revTCA in the following), which was introduced in order to correct for the self-interaction error of the correlation energy functional for hydrogenoid atoms. We also tested combinations of TCA correlation with two of the abovementioned exchange forms, leading to the (viii) PBEsolTCA and (ix) SOGGATCA functionals.

Bulk moduli were obtained from single-point energy calculations of the primitive unit cell equilibrium volumes of the systems, and the data obtained were fitted to a Birch–Murnaghan equation of state [37, 38].

Cohesive energies were obtained as the difference between the sum of the ground-state energies of the n isolated atoms (E_{atom}) of the solid and the total equilibrium lattice energy (E_{solid}):

$$\epsilon_{coh} = \frac{1}{n}[\sum_{atoms} E_{atom} - E_{solid}]. \qquad (1)$$

Similarly to previous works [4, 30], the basis sets used for the isolated atoms and solids were different in some cases. More precisely, the following basis sets were used for isolated atom calculations: 6-31G for Li and Al 6-311G* for the cations of LiF, LiCl, NaF, NaCl, and MgO, as well as the boron atom of BN and BP; Ahlrichs VTZ for Cu; LANL2DZ for Rh; and LANL2TZ for Pd and Ag. In all other cases, the basis sets for the periodic and atomic calculations are the same.

Results and discussion

Tables S1 and 1 present equilibrium lattice constants and corresponding mean signed errors (MSEs) and mean unsigned

Table 1 Computed errors in equilibrium lattice constants (Å) obtained using different exchange-correlation functionals. Lowest errors with respect to the experimental data are shown in boldface

	3 metals		9 semiconductors		5 ionic solids		4 transition metals		21 solids	
	MSE	MUE	MSE	MUE	MSE	MUE	MSE	MUE	MSE	MUE
SVWN5	−0.080	0.080	−0.018	0.020	−0.068	0.068	−0.038	0.039	−0.042	0.044
SRC04	−0.081	0.081	−0.014	0.018	−0.064	0.064	−0.037	0.040	−0.040	0.042
PBE	0.010	0.017	0.067	0.067	0.103	0.103	0.067	0.067	0.067	0.068
PBEsol	−0.008	0.023	0.021	0.023	0.033	0.033	0.005	0.019	0.017	0.025
TCA	0.027	0.027	0.074	0.074	0.126	0.126	0.078	0.078	0.080	0.080
PBEsolTCA	0.008	0.018	0.018	0.023	0.058	0.058	0.003	**0.018**	0.024	0.030
revTCA	0.066	0.066	0.096	0.098	0.211	0.211	0.103	0.103	0.120	0.121
SOGGA	−0.009	0.018	**0.009**	**0.017**	**0.024**	**0.029**	0.019	0.034	**0.012**	**0.023**
SOGGATCA	**−0.005**	**0.014**	0.016	0.022	0.048	0.048	**0.002**	0.019	0.018	0.026

errors (MUEs) computed from the experimental data for the test set of 21 solids mentioned in "Computational details," obtained with the nine exchange-correlation functionals considered in this work. Generally, excellent agreement with previously published GTO data is observed, and general well-known trends are obtained from the computed MSEs: LDAs (SVWN5 or SRC04) underestimate the lattice constants (except for SiC), while GGAs generally overestimate them (except for Na). From the computed MUE data (see Table 1), the best performing functionals are: SOGGA > PBEsol ~ SOGGATCA > PBEsolTCA > SVWN5 ~ SRC04 > PBE > TCA >> revTCA. The computed MUEs and MSEs are in excellent agreement with previously published works [4–6, 10, 15, 31, 32, 30] for the functionals that they have in common. In particular, we confirm that the SOGGA and PBEsol exchanges give excellent performance, as already found with smaller [6] and larger [15] test sets. With LDAs, the largest errors are obtained for metals, while GGAs mostly fail with ionic solids. Since the TCA functional performs slightly less well than PBE for equilibrium lattice determination, combining the TCA correlation with the SOGGA or PBEsol exchange does not improve the results compared to those of the original GGAs. Nevertheless, it should however be noted that the performances of the SOGGATCA (MUE of 0.026 Å) and PBEsolTCA (MUE of 0.030 Å) functionals are very close to (or even better than) those of meta-GGAs such as TPSS or revTPSS, as well as that of a parametrized GGA such as N12 that is fitted to perform well for both energetics and structures, with reported MUEs for a slightly smaller test set (18 solids) of 0.054, 0.034, 0.021 Å , respectively [15]. On the other hand, the parametrized HTBS functional of Haas et al. [13] has a MUE of 0.054 Å for a larger test set (60 solids), and was also designed to do well for both energetics and structures, meaning that the results obtained when combining the TCA correlation with exchange forms biased towards solids (such as PBEsol or SOGGA) are encouraging.

Bulk moduli and related errors are presented in Tables S2 and 2, respectively. Note that, due to severe convergence problems in the SCF in the cases of BN and Li, only data for the remaining 19 solids are reported in Table S2. In addition, due to the large uncertainty in the experimental bulk modulus of GaN, it is excluded from the statistical data of Table 2. The general agreement with previously published data [4–6, 10, 13, 30, 32] is good. Overall, for functionals that clearly underestimate (SVWN5 and SRC04) and overestimate (PBE, TCA and revTCA) lattice parameters, computed bulk moduli are overestimated and underestimated, respectively. On the other hand, the other functionals considered (PBEsol, PBEsolTCA, SOGGA, and SOGGATCA) tend to overestimate this property. In addition, from the computed MUEs of the 18 solids, the best-performing functionals are: PBE > TCA > SOGGATCA ~ PBEsolTCA > revTCA > SOGGA ~ PBEsol > SRC04 > SVWN5. The performances of the PBEsolTCA and SOGGATCA functionals, for example (MUEs of 12.3 and 12.9 GPa, respectively), are similar to those of the HTBS functional (MUE of 14.7 GPa on a test set of 60 solids) [13], which has recently been shown to be at least as good for this property [13] as WC [10], a GGA specifically developed for solids. Surprisingly, we could not reproduce the good performace of the PBEsol functional for the bulk modulus calculation mentioned in previous works [16, 30], except when transition metals were excluded from the solid test set. In this case, the PBEsol and PBE MUEs are much closer: 8.6 and 6.8 GPa, respectively.

Finally, we consider the cohesive energy data, which are reported in Table S3 along with corresponding errors with respect to the experimental data in Table 3. As is well known, the standard LDA overbinds strongly. This failure is largely corrected by SRC04, which reduces the MUE by 33 %. The performance of SRC04 is not far from those of SOGGA and PBEsol, while the other GGAs generally perform better, underbinding in some cases (TCA and revTCA) but overbinding most of the time (all other functionals). The

Table 2 Computed errors on bulk moduli (GPa) obtained using different exchange-correlation functionals. Lowest errors with respect to the experimental data are shown in boldface

	2 metals		7 semiconductors		5 ionic solids		4 transition metals		18 solids	
	MSE	MUE	MSE	MUE	MSE	MUE	MSE	MUE	MSE	MUE
SVWN5	6.4	6.4	7.4	9.5	14.9	14.9	58.6	58.6	20.8	21.6
SRC04	6.6	6.6	7.1	9.2	13.7	13.7	57.5	57.5	20.1	20.9
PBE	2.6	2.6	−9.8	9.8	−3.1	4.2	4.0	11.4	**−3.5**	**7.8**
PBEsol	5.7	5.7	6.3	11.6	1.7	5.5	34.6	34.6	11.2	14.4
TCA	1.1	1.1	−11.8	12.2	−4.1	5.3	**−1.5**	**10.7**	−5.9	8.7
PBEsolTCA	6.6	6.6	5.4	10.1	−1.0	**3.0**	33.2	33.1	9.9	12.9
revTCA	**0.8**	**1.0**	−16.7	16.7	−9.3	9.3	−13.1	16.2	−11.9	12.8
SOGGA	7.3	7.3	3.8	6.0	2.3	5.6	43.3	43.3	12.5	14.4
SOGGATCA	6.0	6.0	**1.8**	**6.0**	**0.6**	4.2	36.8	36.8	9.7	12.3

best results are obtained at the PBE level, closely followed by TCA. This leads to a significant improvement in the computed data when going from PBEsol to PBEsolTCA, and from SOGGA to SOGGATCA. From the computed MUEs, the best-performing functionals for the cohesive energy determination are then: PBE > TCA > PBEsolTCA > SOGGATCA > revTCA > PBEsol > SOGGA > SRC04 > SVWN5. If we consider a smaller test set of eight solids (SSCE8), commonly used in previous papers [4, 6, 15], the excellent performances of PBE, PBEsolTCA, and SOGGATCA are confirmed. We note that the computed MUE values obtained at the PBEsolTCA/SSCE8 or SOGGATCA/SSCE8 levels (0.20 and 0.23 eV/atom, respectively) are very close to the 0.13 eV/atom value very-recently reported by Peverati and Truhlar, obtained with their highly parametrized N12 functional [15], which was developed to provide good accuracy for key structural and energetic properties of solids and molecules.

Finally, it is interesting to mention that for all functionals, the largest errors originate from the group of ionic compounds for both lattice constants and cohesive energy calculations, while bulk moduli of transition metals clearly show the worst agreement with the experimental data. The cohesive energy trends are in line with the recently reported performances of different functionals for energetic data from different systems (atoms, molecules, and different groups of solids) [21].

Conclusions

In this work, we tested the performances of nine exchange-correlation functionals for solids, extending previous work for molecules carried out with two parameter-free correlation functionals (TCA and revTCA). Two local functionals and seven GGAs were considered for the prediction of the equilibrium lattice constants, bulk moduli, and cohesive energies of a test set of 21 solids, including metals, semiconductors, ionic solids, and transition metals, when possible. All calculations were performed with reference GTO basis sets in order to obtain a straightforward comparison

Table 3 Computed errors in cohesive energies (eV/atom) obtained using different exchange-correlation functionals. Lowest errors with respect to the experimental data are shown in boldface. The SSCE8 test set is that of [4] and includes only C, Si, SiC, Ge, NaCl, NaF, LiCl, and LiF

	3 metals		9 semiconductors		5 ionic solids		4 transition metals		21 solids		SSCE8	
	MSE	MUE	MSE	MUE	MSE	MUE	MSE	MUE	MSE	MUE	MSE	MUE
SVWN5	0.53	0.53	1.10	1.10	0.56	0.56	1.30	1.30	0.93	0.93	0.75	0.75
SRC04	0.26	0.36	0.63	0.63	0.32	0.32	1.15	1.15	0.60	0.62	0.41	0.41
PBE	0.12	0.18	0.17	0.23	**−0.03**	**0.09**	**0.00**	**0.30**	**0.09**	**0.20**	**0.02**	**0.12**
PBEsol	0.31	0.31	0.59	0.59	0.15	0.15	0.68	0.68	0.47	0.47	0.31	0.31
TCA	**−0.06**	**0.10**	**−0.13**	**0.18**	−0.13	0.13	−0.28	0.42	−0.15	**0.20**	−0.19	0.19
PBEsolTCA	0.21	0.30	0.30	0.38	**−0.01**	**0.07**	0.46	0.51	0.24	0.32	0.06	0.20
revTCA	−0.18	0.18	−0.34	0.34	−0.31	0.31	−0.72	0.72	−0.38	0.38	−0.39	0.39
SOGGA	0.42	0.42	0.66	0.66	0.15	0.15	0.82	0.82	0.53	0.53	0.35	0.35
SOGGATCA	0.22	0.30	0.34	0.44	**0.04**	**0.08**	0.53	0.54	0.29	0.35	0.09	0.23

with previously published data. The effect of the choice of the exchange contribution to the total exchange correlation was also tested by combining the TCA correlation with two exchange functionals designed for solids (SOGGA and PBEsol), leading to the SOGGATCA and PBEsolTCA functionals.

For lattice constants, we confirmed the excellent performance of SOGGA, and noted that the TCA correlation combined with the PBE exchange provides data close to the results from PBE. Although combining the TCA correlation with the SOGGA or PBEsol exchange does not improve on the original SOGGA and PBEsol functionals, the resulting functionals still provide good accuracy, with errors similar to those of N12, a highly parametrized functional that was designed to perform well for key structural and energetic properties of solids and molecules.

For the bulk moduli, in general, clear underestimation of the lattice parameters (as obtained by the LDAs) led to significant overestimation of the bulk moduli, and vice versa. We also found that the accuracy of the PBEsolTCA results is similar to those yielded by parametrized functionals designed for energetics and structures, such as HTBS.

Finally, concerning the cohesive energies of solids, we have found that the standard LDA gives values that are too large—an error which is strongly reduced by the local SRC04 functional. This confirms similar improvements that were previously found for molecules [39, 40]. The GGAs generally performed better; sometimes overbinding, but in some cases (TCA and revTCA) underbinding. In particular, we found that the performances of TCA were very close to those of PBE, which is currently a reference GGA functional for calculations of this property. Consequently, combining the TCA correlation with the PBEsol or the SOGGA exchange in the PBEsolTCA and SOGGATCA functionals, respectively, led to some significant improvements in the computed energetic data with respect to the original PBEsol and SOGGA functionals. For instance, the PBEsolTCA and SOGGATCA errors are very close to the one obtained with the N12 functional mentioned above, which was recently found to be one of the best-performing functionals for cohesive energy calculations of a test set of eight solids among the 15 GGAs, 4 meta-GGAs, and 1 hybrid tested [15].

To sum up, we found that the previously noted good accuracy of the parameter-free TCA functional for molecules also held for solids, as long as a modified form of the exchange functional that was more biased towards solids than PBE was taken into account. This was the case for the PBEsol exchange, which meant that the PBEsolTCA functional performed well overall for the three key structural and energetic properties considered here.

Acknowledgments Thanks are due to Prof. Csonka (Budapest University of Technology and Economics) and Dr. Vydrov (Massachusetts Institute of Technology) for fruitful discussions, and to Dr. John Jaffe (Pacific Northwest National Laboratory) for providing the Na basis set. We also wish to acknowledge the ANR agency for funding (project DinfDFT ANR. 2010 BLANC no. 0425 02).

References

1. Kohn W, Sham LJ (1965) Phys Rev 140:A1133–A1138
2. Perdew JP, Ruzsinszky A, Constantin LA, Sun J, Csonka GI (2009) J Chem Theory Comput 5:902–908
3. Corá F, Alfredsson M, Mallia G, Middlemiss DS, Mackrodt WC, Dovesi R, Orlando R (2004) Struct Bond 113:171
4. Staroverov VN, Scuseria GE, Tao J, Perdew JP (2004) Phys Rev B 69:075102
5. Perdew JP, Ruzsinszky A, Csonka GI, Constantin LA, Sun J (2009) Phys Rev Lett 103:026403
6. Zhao Y, Truhlar DG (2008) J Chem Phys 128:184109
7. Peverati R, Truhlar DG (2012) J Phys Chem Lett 3:117–124
8. Vitos L, Johansson B, Kollár J, Skriver HL (2000) Phys Rev B 62:10046–10050
9. Mattsson AE, Armiento R, Paier J, Kresse G, Wills JM, Mattsson TR (2008) J Chem Phys 128:084714
10. Wu Z, Cohen RE (2006) Phys Rev B 73:235116
11. Madsen GKH (2007) Phys Rev B 75:195108
12. Perdew JP, Ruzsinszky A, Csonka GI, Vydrov OA, Scuseria GE, Constantin LA, Zhou X, Burke K (2008) Phys Rev Lett 100:136406
13. Haas P, Tran F, Blaha P, Schwarz K (2011) Phys Rev B 83:205117
14. Ruzsinszky A, Csonka GI, Scuseria GE (2009) J Chem Theory Comput 5:763–769
15. Peverati R, Truhlar DG (2012) J Chem Theory Comput 8:2310–2319
16. Fabiano E, Constantin LA, Della Sala F (2010) Phys Rev B 82:113104
17. Fabiano E, Constantin LA, Della Sala F (2012) Int J Quantum Chem (in press). doi:10.1002/qua.24042
18. Fabiano E, Constantin LA, Della Sala F (2011) J Chem Theory Comput 7:3548–3559
19. Perdew JP, Burke K, Ernzerhof M (1996) Phys Rev Lett 77:3865–3868
20. Vela A, Medel V, Trickey SB (2009) J Chem Phys 130:244103
21. Schimka L, Harl J, Kresse G (2011) J Chem Phys 134:024116
22. Haas P, Tran F, Blaha P, Pedroza LS, da Silva AJR, Odashima MM, Capelle K (2010) Phys Rev B 81:125136
23. Csonka GI, Perdew JP, Ruzsinszky A (2010) J Chem Theory Comput 6:3688–3703
24. Tognetti V, Cortona P, Adamo C (2008) J Chem Phys 128:034101
25. Tognetti V, Cortona P, Adamo C (2008) Chem Phys Lett 460:536–539
26. Tognetti V, Adamo C, Cortona P (2010) Interdiscip Sci Comput Life Sci 2:163–168
27. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA Jr, Peralta JE, Ogliaro F, Bearpark M, Heyd J, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Parandekar

PV, Mayhall NJ, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2009) Gaussian development version, revision H.10. Gaussian, Inc., Wallingford

28. Kudin KN, Scuseria GE (2000) Phys Rev B 61:16440
29. Perdew JP, Ruzsinszky A, Csonka GI, Vydrov OA, Scuseria GE, Constantin LA, Zhou X, Burke K (2009) Phys Rev Lett 102:039902
30. Csonka GI, Perdew JP, Ruzsinszky A, Philipsen PHT, Lebègue S, Paier J, Vydrov OA, Ángyán JG (2009) Phys Rev B 79:155107
31. Heyd J, Peralta JE, Scuseria GE, Martin RL (2005) J Chem Phys 123:174101
32. Paier J, Marsman M, Hummera K, Kresse G, Gerber IC, Ángyán JG (2006) J Chem Phys 124:154709
33. Dirac PAM (1930) Proc Cambridge Phil Soc 26:376
34. Vosko SH, Wilk L, Nusair M (1980) Can J Phys 58:1200
35. Hammer B, Hansen LB, Nørskov JK (1999) Phys Rev B 59:7413–7421
36. Ragot S, Cortona P (2004) J Chem Phys 121:7671–7680
37. Birch F (1978) J Geophys Res 83:1257–1268
38. Murnaghan FD (1944) Proc Natl Acad Sci USA 30:244–247
39. Tognetti V, Cortona P, Adamo C (2007) Chem Phys Lett 439:381–385
40. Tognetti V, Adamo C, Cortona P (2007) Chem Phys 337:161–165