Erratum: Tests of a ladder of density functionals for bulk solids and surfaces [Phys. Rev. B 69, 075102 (2004)]

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(Received 8 December 2008; published 31 December 2008)

DOI: 10.1103/PhysRevB.78.239907 PACS number(s): 71.15.Mb, 71.15.Ap, 61.50.Ah, 62.20.D−, 99.10.Cd

In most of the numbered equations, the symbols V and V_0 can refer either to the volume per primitive unit cell or to the volume per atom (so long as the energy is defined respectively). But Eq. (18), which gives an estimate of the zero-point anharmonic expansion (ZPAE) that must be subtracted from the experimental low-temperature lattice constant to obtain the static-lattice value, requires the volume per atom.[1] When calculating the ZPAE of Eq. (18) for a solid whose primitive cell contains two atoms (a nonmetal), we inadvertently used the volume per primitive cell. As a result, the ZPAE corrections incorporated into the parenthesized experimental lattice constants of the ten nonmetals in Table III were underestimated by a factor of 2. The revised experimental a_0 values adjusted for ZPAE appear in the following table in bold. The static-lattice constants of the other eight solids (all metals) are not changed, but we include them for completeness and ease of reference along with the experimental Debye temperatures of Refs. 66 and 67.

Solid	Θ_D, K	a_0^{expt}(0 K)	a_0^{expt}(−ZPAE)[a]
Li	344	3.477	3.451
Na	158	4.225	4.210
K	91	5.225	5.212
Al	428	4.032	4.020
C	2230	3.567	**3.544**
Si	640	5.430	**5.416**
SiC	1232	4.358	**4.340**
Ge	370	5.652	**5.640**
GaAs	344	5.648	**5.638**
NaCl	321	5.595	**5.566**
NaF	492	4.609	**4.579**
LiCl	422	5.106	**5.074**
LiF	732	4.010	**3.964**
MgO	946	4.207	**4.188**
Cu	343	3.603	3.596
Rh	480	3.798	3.793
Pd	274	3.881	3.877
Ag	225	4.069	4.064

[a]Revised values are in bold.

This amendment affects the statistics of errors of the density-functional lattice constants for all 18 solids relative to the experimental ZPAE-corrected values (i.e., the m.e., m.a.e., and m.a.r.e. values in parentheses at the bottom of Table III). The revised statistics is as follows.

	a_0^{LSDA}	a_0^{PBE}	a_0^{PKZB}	a_0^{TPSS}
m.e. (Å)	(−0.051)	(0.070)	(0.096)	(0.056)
m.a.e. (Å)	(0.053)	(0.071)	(0.096)	(0.057)
m.a.r.e. (%)	(1.20)	(1.54)	(2.07)	(1.21)

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No other results or conclusions are changed by this erratum, although the errors of LSDA for lattice constants are slightly reduced, while those for PBE, PKZB, and TPSS are slightly increased. V.N.S. and J.P.P. thank Fabien Tran for pointing out this error.

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[1] A relevant discussion is footnote 10 of Chapter 23 in: N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart, and Winston, New York, 1976).