Erratum: Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces [Phys. Rev. Lett. 100, 136406 (2008)]

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Table I of this Letter and Table SI of its Supplementary Information require small corrections to the corrected experimental values of the lattice constants for the nonmetals.

The errors of the density-functional lattice constants in Table I were deviations from corrected experimental values, where the corrections removed the finite-temperature and zero-point anharmonic expansion (ZPAE) effects. The ZPAE corrections were taken from Ref. [28] and based on Eq. (18) of Ref. [28], i.e., on Appendix A of A. B. Alchagirov *et al.*, Phys. Rev. B **63**, 224115 (2001), in which ε is the energy per atom and v_0 is the volume per atom. But Ref. 28 inadvertently used the volume per unit cell, which is twice the volume per atom for the semiconductors and ionic crystals. Thus, the ZPAE corrections for these solids in Ref. [28] and in our article were only half what they should have been. Parts of Table I (with errors in units of 0.01 Å) of our article should be corrected as follows:

Class	LSDA	PBE	TPSS	PBEsol
Mean error				
5 semiconductors	−0.3	8.6	7.0	3.7
5 ionic solids	−6.9	10.1	8.3	3.5
Total	−4.9	7.3	6.0	1.9
Mean absolute error				
5 semiconductors	0.9	8.6	7.0	3.7
5 ionic solids	6.9	10.1	8.3	3.5
Total	5.1	7.4	6.0	2.9

The corrected experimental lattice constants for the 4 simple metals and 4 transition metals in Table I are unaffected. No conclusion is changed by this erratum, although the improvement of PBEsol relative to LSDA is slightly reduced. Some lattice constants (in Å) from the "Expt.-ZPAE" column of Table S1 of the Supplementary Information (EPAPS PRLTAO-100-016814) should be corrected as follows: 3.544 (C), 5.416 (Si), 4.340 (SiC), 5.640 (Ge), 5.638 (GaAs), 5.566 (NaCl), 4.579 (NaF), 5.074 (LiCl), 3.964 (LiF), and 4.188 (MgO).

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