Erratum: Calculation of the lattice constant of solids with semilocal functionals [Phys. Rev. B 79, 085104 (2009)]

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For several solids, the calculated equilibrium lattice constants a_0 (Table I) were not well converged with respect to all parameters used for the calculations. As mentioned in the paper, the results were converged with respect to the number of **k** points for the integration in the Brillouin zone and the value of $R_{\mathrm{MT}}^{\mathrm{min}}K_{\mathrm{max}}$ which determines the size of the basis set. However, for some solids, the choice of the radius of the muffin-tin sphere R_{MT} (which influences the linearization of the radial wave function) and the size of the grid for the integrations using the fast Fourier transform revealed to be inadequate. The new results which differ by more than ~0.005 Å with respect to the older are given in the following table. None of the conclusions of the paper are affected by these changes.

P.B. thanks Gábor I. Csonka for pointing out the inaccuracy of some results.

TABLE I. Recalculated equilibrium lattice constants a_0 (in Å) of 14 solids. The updated statistical quantities me, mae, mre, and mare were calculated with the whole set of 60 solids. See the caption of the original table for more details.

Solid	LDA	SOGGA	PBEsol	WC	AM05	TPSS	PBE	Expt.
Rb (A2)	5.372	**5.592**	**5.570**	5.608	5.676	5.749	5.668	5.577(5.585)
Pd (A1)	3.840	**3.859**	**3.875**	**3.884**	**3.870**	3.905	3.942	3.876(3.881)
Ge (A4)	**5.625**	**5.656**	5.678	5.681	5.683	5.724	5.763	5.639(5.652)
Sn (A4)	**6.473**	6.513	6.540	6.541	6.557	6.615	6.655	6.474(6.482)
LiF (B1)	3.911	4.003	4.006	4.012	4.038	4.039	4.068	3.960(4.010)
LiCl (B1)	4.965	5.042	**5.063**	**5.069**	5.118	5.115	5.150	5.072(5.106)
NaCl (B1)	5.465	5.594	5.605	5.623	5.682	5.704	5.700	5.565(5.595)
MgS (B1)	5.132	**5.169**	**5.184**	**5.189**	**5.191**	5.224	5.231	5.182(5.202)
HfN (B1)	4.472	**4.497**	**4.506**	**4.511**	**4.501**	4.541	4.550	4.512(4.520)
AlAs (B3)	**5.630**	**5.663**	5.676	5.676	5.680	5.706	5.729	5.646(5.658)
GaAs (B3)	5.607	**5.642**	**5.662**	**5.664**	5.670	5.715	5.747	5.637(5.648)
InP (B3)	5.825	**5.862**	**5.880**	**5.882**	5.886	5.951	5.961	5.856(5.866)
InAs (B3)	**6.027**	**6.065**	6.088	6.091	6.102	6.161	6.187	6.044(6.054)
CeO_2 (C1)	5.356	**5.379**	**5.394**	**5.399**	**5.397**	5.439	5.459	5.393(5.401)
me (Å)	−0.060	−0.016	−0.007	−0.001	0.003	0.034	0.049	
	(−0.072)	(−0.028)	(−0.019)	(−0.013)	(−0.009)	(0.022)	(0.037)	
mae (Å)	0.060	0.029	0.028	0.029	0.033	0.045	0.053	
	(0.072)	(0.032)	(0.029)	(0.028)	(0.032)	(0.037)	(0.045)	
mre (%)	−1.37	−0.42	−0.21	−0.07	−0.03	0.66	1.02	
	(−1.63)	(−0.69)	(−0.48)	(−0.34)	(−0.31)	(0.38)	(0.74)	
mare (%)	1.37	0.68	0.64	0.64	0.74	0.95	1.14	
	(1.63)	(0.76)	(0.67)	(0.64)	(0.73)	(0.79)	(0.96)	

