PHYSICAL REVIEW B, VOLUME 65, 119901(E)

Erratum: Structure and energetics of stoichiometric TiO_2 anatase surfaces [Phys. Rev. B 63, 155409 (2001)]

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(Published 15 February 2002)

DOI: 10.1103/PhysRevB.65.119901 PACS number(s): 68.03.Cd, 68.35.Bs, 71.15.Nc, 71.15.Mb, 99.10.+g

An error was found in one of the beta functions of the Vanderbilt-like pseudopotential used for titanium within the PBE approximation. We repeated the calculations using the correct Ti pseudopotential, and found only small variations in the results. Moreover, all the conclusions of our work remain unchanged.

In particular: (i) the bulk equilibrium parameters of rutile and anatase do not change, anatase is still found to be more stable than rutile, and the difference in cohesive energy between the two phases is still 0.10 eV/TiO_2; (ii) the parameters describing the relaxation of the various surfaces are the same; (iii) the surface formation energies E^{surf}, calculated with the correct pseudopotential, are reported in Table I. These values are systematically smaller than the previously published ones by ~ 0.06 J/m^2, so that the relative stability of different surfaces is not significantly affected.

As already outlined in the paper, it is difficult to establish the absolute accuracy of our calculated values of E^{surf}, nevertheless we expect the error to be systematic to all the surfaces studied. Since the conclusions of our paper were based on the analysis of the relative values of E^{surf} for different surfaces, they are not affected by this error.

We thank Paolo Giannozzi for pointing out the error in the pseudopotential.

TABLE I. Comparison between our previously published surface formation energies (E^{surf}_{old}), with those calculated using the correct pseudopotential (E^{surf}_{new}). All values are in J/m^2. Notice that E^{surf}_{old} was denoted E^{rel}_{PBE} in Table II of our paper.

	Rutile	Anatase					
	(110)	(101)	(100)	(001)	$(103)_f$	$(103)_s$	(110)
E^{surf}_{old}:	0.35	0.49	0.58	0.98	0.90	0.99	1.15
E^{surf}_{new}:	0.31	0.44	0.53	0.90	0.83	0.93	1.09