Erratum: Analytic many-body potential for InAs/GaAs surfaces and nanostructures: Formation energy of InAs quantum dots [Phys. Rev. B 77, 235303 (2008)]

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In our paper we have proposed a parametrization of the Abell-Tersoff potential for In, Ga, As, InAs and GaAs. This is to report corrections to the results presented there. Specifically, surface energies of non-stoichiometric surfaces, quoted for a specific value of the arsenic chemical potential, were in error due to inconsistent usage of the As chemical potential. The correct surface energies as calculated with the previously published parametrization T1,[1] T2,[2] T3,[3] T4,[4] T5,[5] T6,[6] T7,[7] and our parametrization (denoted as T9) are reported in Tables I and II, replacing the according entries in Tables VII to X of our paper. The surface energies of stoichiometric surface reconstructions and the relaxation differences ($\|F_0\|$ and $\langle \Delta r \rangle$) given in these original Tables are not shown here as they are not affected by the inconsistent usage of the As chemical potential. The correct surface energies of our parametrization (T9) deviate from the DFT values since the inconsistent usage of the As chemical potential obstructed the fitting of parameters. In extension to Sec. III.C and Sec. III.D of our paper, we note that the relaxation of surface slabs was limited to 100 iterations and that T5 referred to a modified version of the parameters from Ref. 5 using $R_{ij}^c = 3.1$ Å and $D_{ij}^c = 0.1$ Å as cutoff parameters for the As-As interaction. These cutoff parameters effectively define a nearest-neighbour scheme in order to reproduce the results for the GaAs bulk phases presented in the original work.[5]

For potential parameters T8,[8] we again report *all* surface energies. Previous results were ambiguous, because the cutoff parameters for the potential T8 had not been provided in Ref. 8. The new results reported in Table IV and V are obtained with the cutoff parameters listed in Table III.

TABLE I. Corrected surface energies γ (meV/Å^2) of GaAs surfaces (to replace the according entries in Table VII and IX of our paper).

	T1	T3	T5	T7	T9
(001)β(2×4)	67.6	47.7	68.4	71.3	18.0
(001)β2(2×4)	68.3	57.6	69.0	72.7	18.2
(113)(2×1)-α	58.2	48.1	74.4	68.4	24.6
(137)	58.1	44.0	67.5	70.3	33.9
(2 5 11)	50.2	39.4	72.8	67.0	33.4
(3 7 15)	49.3	39.2	72.2	66.5	34.2

TABLE II. Corrected surface energies γ (meV/Å^2) of InAs surfaces (to replace the according entries in Table VIII and X of our paper).

	T2	T4	T6	T7	T9
(001)β2(2×4)	63.6	64.8	41.7	79.5	13.5
(113)(2×1)-α	54.0	57.9	31.5	70.7	17.8
(137)	50.7	54.7	27.5	70.3	24.9
(3 7 15)	44.8	48.2	24.0	66.3	25.7

TABLE III. Cutoff parameters used to repeat the calculations for T8.

	Ga–Ga	As–As	In–In	Ga–As	In–As
R_{ij}^c (Å)	2.95	3.1	3.5	3.1	3.2
D_{ij}^c (Å)	0.15	0.1	0.1	0.2	0.1

TABLE IV. Corrected bulk properties using T8 with original cutoff parameters (to replace according entries in Table V and VI of our paper).

	GaAs (CsCl)	InAs (NaCl)	InAs (CsCl)
a_0 (Å)	3.1940	5.4348	3.5574
E_{coh} (eV)	5.7827	7.4804	7.5200
B (GPa)	671.55	106.71	662.35

TABLE V. Corrected surface quantities of GaAs and InAs surfaces using parameters T8 (to replace the according entries in Table VII to X of our paper).

	γ (meV/Å^2)	$\|F_0\|$ (eV/Å)	$\langle \Delta r \rangle$ (Å)
GaAs (001)$\alpha(2\times4)$	101.6	2.929	0.102
GaAs (001)$\beta(2\times4)$	31.5	1.320	0.104
GaAs (001)$\beta2(2\times4)$	32.1	0.731	0.106
GaAs (110)(cleavage)	21.9	0.538	0.100
GaAs (113)(2×1)-α	30.8	0.562	0.0781
GaAs (137)	31.1	0.587	0.0813
GaAs (2 5 11)	28.7	0.621	0.0886
GaAs (3 7 15)	29.1	0.791	0.105
InAs (001)$\alpha2(2\times4)$	51.8	10.58	0.149
InAs (001)$\beta2(2\times4)$	9.8	8.853	0.152
InAs (110)(cleavage)	54.1	0.249	0.108
InAs (113)(2×1)-α	16.5	8.048	0.107
InAs (137)	24.0	8.588	0.0926
InAs (3 7 15)	26.1	7.537	0.106

In Table IV we report the results for those bulk systems that were affected by our previous choice of cutoff parameters to replace the according entries in Tables V and VI of our paper. All other bulk and defect properties remain unchanged. The surface quantities using the above set of cutoff parameters are also reported here to replace the according entries for T8 in Tables VII to X of our paper.

We also note the following corrections to misprinted table entries in our paper: The correct values (in GPa) of c_{11} for T7, T8, and T9 in Table V in our paper are 124.01, 117.74, and 118.80, respectively. The correct values for $\|F_0\|$ (in eV/Å) on GaAs(001)$\alpha(2\times4)$ using T7 (Table VII) and on InAs(110) using T4 (Table VIII) are 1.31 and 0.783, respectively.

The aspects of our work referenced by Titantah *et al.*[9] are not affected by this erratum.

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