

Erratum: *Ab initio* derived augmented Tersoff potential for silicon oxynitride compounds and their interfaces with silicon [Phys. Rev. B 73, 155329 (2006)]

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Two misprints have been detected in both Eqs. (12) and (13). This is their correct expression:

$$E = \frac{1}{2} \sum_{i \neq j} V_{ij} + \sum_I N_I E_I^0. \quad (12)$$

$$E = \frac{1}{2} \sum_{i \neq j} V_{ij} + \sum_I N_I E_I^0 + \sum_i E_i^c. \quad (13)$$

In the last paragraph of Section III (Augmented Tersoff Potential for SiONH Systems), the following sentence fragment must be erased: “and $\text{sign}(f_s(z)) = \text{sign}(z)$.”

In Table II the values of some parameters of the ZRL potential were reported incorrectly. For the sake of clarity, here we report the entire Table II with the corrected values in bold.

In Table XIII (Appendix A) one parameter of the α -ZRL potential was reported incorrectly: for nitrogen the correct value of n_I is 2.42395 (instead of 2.42635).

We are grateful to Simone Meloni and Matthias Posselt for pointing out oversights in the text.

TABLE II. Comparison of parameters of the Original and ZRL potentials (see text). Values are in eV, Å, and Å⁻¹

Parameter	Silicon		Oxygen		Nitrogen		Hydrogen	
	Original	ZRL	Original	ZRL	Original	ZRL	Original	ZRL
A_I	1830.8	1830.79	3331	3331.06	6368.14	6368.21	86.7120	86.9235
B_I	471.18	471.195	261.2	260.477	511.760	511.205	43.5310	42.9815
λ_I	2.4799	2.62392	5.36	3.78336	5.43673	5.60181	3.7879	3.8593
μ_I	1.7322	1.88891	2.68	3.34402	2.70000	3.16170	1.9800	1.97047
R_I	2.70	2.44809	2.70	2.26069	1.80	1.75256	0.80	0.77985
S_I	3.00	3.08354	3.00	3.31294	2.10	2.41523	1.00	0.88641
β_I	1.0999×10^{-6}	1.0999×10^{-6}	2	1.0027	5.2938×10^{-3}	4.4422×10^{-3}	4	4
n_I	0.78734	0.78766	1	3.98638	1.33041	2.42635	1	1.00921
m_I	3	3	1	1	1	1	1	1
c_I	1.0039×10^5	1.0039×10^5	0	0 ^a	2.03120×10^4	2.2955×10^4	0	0
d_I	16.217	16.21701	1	1	25.5103	24.78674	1	1
h_I	-0.59826	-0.59784	0	-0.52909	-0.56239	-0.45450	1	0.96783
$\chi_{Si,I}$	1	1	1	1	0.67	1	0.78	1
$\chi_{O,I}$	1	1	1	1	1	1	1	1
$\chi_{N,I}$	0.67	1	1	1	0	1	0.76	1
$\chi_{H,I}$	0.78	1	1	1	0.76	1	1	1

^aAlthough not restrained to zero, the value obtained from fitting was negligible.