# Erratum: Interatomic potentials for hydrogen in $\alpha$–iron based on density functional theory [Phys. Rev. B 79, 174101 (2009)]

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The interpolating function between the Biersack and Ziegler universal screened-Coulomb form and the cubic spline fit was mistyped in Eq. (2) in the original paper as an exponential rather than a polynomial. The correct Fe–H two-body function should read

$$\phi_{\mathrm{FeH}} = \begin{cases} \dfrac{Z_{\mathrm{Fe}} Z_{\mathrm{H}} q_e^2}{r} \Phi\left(\dfrac{r}{r_s}\right) & \text{for } r < r_1, \\ B_0 + B_1 r + B_2 r^2 + B_3 r^3 + B_4 r^4 + B_5 r^5 & \text{for } r_1 \leqslant r \leqslant r_2, \\ \displaystyle\sum_{i=1}^{N^{\phi}} a_i^{\phi} (r_i^{\phi} - r)^3 H(r_i^{\phi} - r) & \text{for } r > r_2, \end{cases} \tag{1}$$

where $Z_{\mathrm{Fe}}$ and $Z_{\mathrm{H}}$ are the atomic numbers of Fe and H, respectively; $q_e$ is the electronic charge; $H(\cdot)$ is the Heaviside step function; $r_s = 0.88534 a_0 / \sqrt{(Z_{\mathrm{Fe}}^{2/3} + Z_{\mathrm{H}}^{2/3})}$ is the screening length, $a_0$ being the Bohr radius; and

$$\Phi(x) = 0.1818 e^{-3.2x} + 0.5099 e^{-0.9423x} + 0.2802 e^{-0.4029x} + 0.02817 e^{-0.2016x}, \tag{2}$$

is the screening function. The square-root in the screening length was inadvertently omitted in the original paper. The knot point $r_4^{\rho_{\mathrm{HFe}}}$ in Table VIII in the original paper should be at 3.0 Å. Finally, the parameters for the interpolating polynomial should be revised as indicated in Table I; all other parameters remain unaltered.[1]

Please note that these corrections only alter the Fe–H two-body interaction for distances below 1.2 Å, a range that is never actually sampled in any of the atomic configurations used in the fitting procedure. The Fe–H two-body interaction in all our configurations is completely described by the cubic splines—the interpolating polynomial and the Biersack-Ziegler form merely provide continuity below 1.2 Å. Hence, our results and conclusions remain unaltered.

TABLE I. Parameters for the interpolating polynomial in Eq. (1). Energies and distances are in eV and Å, respectively.

| Parameter | Potential A | Potential B |
|---|---|---|
| $B_0$ | 1242.1709168218642 | 1242.154614241987 |
| $B_1$ | −6013.566711223783 | −6013.4610429013765 |
| $B_2$ | 12339.540893927151 | 12339.275191444543 |
| $B_3$ | −12959.66163724488 | −12959.339514470237 |
| $B_4$ | 6817.850021676971 | 6817.662603221567 |
| $B_5$ | −1422.1723964897117 | −1422.130403271231 |

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[1] Updated potential files formatted for use with LAMMPS may be downloaded from http://www.princeton.edu/mae/people/faculty/carter/homepage/research/potentials

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