Erratum: Interatomic potentials for hydrogen in α–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

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

where Z_{Fe} and Z_{H} are the atomic numbers of Fe and H, respectively; q_e is the electronic charge; $H(\cdot)$ is the Heaviside step function; $r_s = 0.88534 a_0/\sqrt{(Z_{\text{Fe}}^{2/3} + Z_{\text{H}}^{2/3})}$ 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 $r_4^{\rho_{\text{HFe}}}$ 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