

Erratum: Repulsive interatomic potentials calculated at three levels of theory [Phys. Rev. A **111**, 032818 (2025)]

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In this erratum, we provide new parameters for the Na-O screening function that had an unphysical value at the limit of infinite distance in the original data set.

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In our paper we developed interatomic repulsive potentials suitable for modeling radiation effects. One of the main results of the article were screening function coefficients for diatoms of all pairs of elements with atomic numbers $Z_1, Z_2 \leq 92$, which were presented in the online supplemental materials and the open access database. These parameters were shown to accurately describe repulsive interatomic interactions at short interatomic distances r in the region where the potential energy for the diatom pair $V(r) > 30$ eV.

The developed pair-specific analytical potentials are formed by multiplying the Coulomb potential

$$V_{\text{Coul}}(r) = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2}{r} \quad (1)$$

(here, $\epsilon_0 = 8.854\,187\,817 \times 10^{-12}$ F/m and r is the interatomic separation distance) with a screening function of the form

$$\phi_{\text{NLH}}(r) = \sum_{i=1}^3 a_i \exp(-b_i r). \quad (2)$$

The pair-specific coefficients a_i, b_i were obtained by fitting to pair-specific quantum mechanical calculations of the diatom energy, with the total electronic energy subtracted such that $V(r = \infty) = 0$.

Due to a numerical fitting issue, the coefficients provided, a_i and b_i , had a problem for the Na-O element pair. For this pair, the previously reported values, $a_3 = 0.004\,99$ and $b_3 = 0$, lead to the feature that $\phi(r)$ does not go to zero when $r \rightarrow \infty$. As a result, the total scattering cross section of this potential is infinite. This is not physically motivated for the reference state that the atoms are neutral when separated far from each other, which is the default assumption when the total electronic energy is subtracted out.

To resolve the issue, we have now redone the fitting for this particular pair, giving a little more weight to the low-energy data points. The new fitting coefficients are provided in Table I. The old and new fits are compared in Fig. 1, which shows that the two fits differ only at large distances, which are not in the repulsive regime.

TABLE I. NLH repulsive potential parameters for the Na-O element pair, obtained by fitting the screening functions to DMol data. E stands for the root-mean-square error of the fit above either 10 (E_{10}) or 30 (E_{30}) eV. Parameters for all the potentials are available in the online open data package [1].

Z_1	Z_2	a_1	a_2	a_3	$b_1 \times \text{\AA}$	$b_2 \times \text{\AA}$	$b_3 \times \text{\AA}$	E_{30} (%)	E_{10} (%)
8	11	0.16691	0.69924	0.13385	27.14183	4.94580	2.70748	1.55	10.45

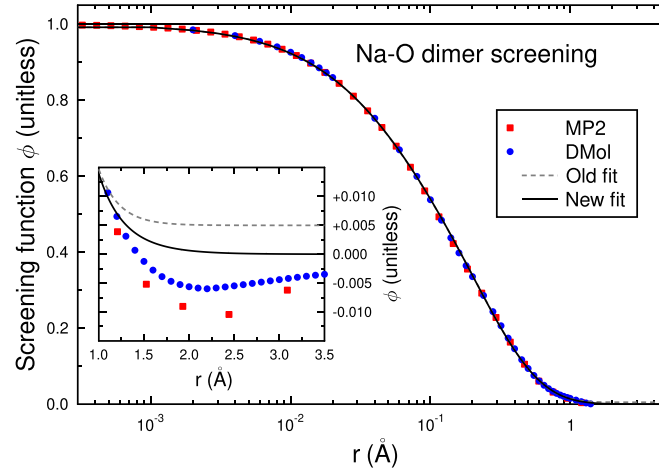


FIG. 1. Comparison of the old and new NLH screening function fits with the quantum mechanical second-order Møller-Plesset (MP2) and DMol data [1]. In the repulsive regime $r \lesssim 1$ Å the two potentials are practically identical. The inset shows that the difference becomes significant only at larger distances which are not any longer in the repulsive regime (the MP2 and DMol data become attractive in this regime).

We have checked that no other element pair provided earlier has the same issue.

We thank Professor Ryan Kingsbury for bringing this issue to our attention.

DATA AVAILABILITY

The open access data set has been updated with these new coefficients [1].

[1] K. Nordlund, S. Lehtola, and G. Hobler, Data sets for the publication “Repulsive interatomic potentials calculated at three levels of theory”, Zenodo, 2025, <https://doi.org/10.5281/zenodo.14172632>.