Erratum: Improved modeling of electrified interfaces using the effective screening medium method [Phys. Rev. B **88**, 155427 (2013)]

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In our original article, we implemented the Green's function only for the vacuum region ($z, z' < z_1$), resulting long-range parts of the local pseudopotential ($V_{\text{loc}}^{\text{LR}}$), and the ion-ion interaction ($E_{\text{ion}}^{\text{LR}}$) assuming that the overlap between the effective screening medium (ESM) and the fictitious Gaussian charges, which are used to describe $V_{\text{loc}}^{\text{LR}}$ and $E_{\text{ion}}^{\text{LR}}$, is negligible. However, we have found that even if the overlap is very small the error is not negligible and as a result, the interaction of a molecule with the ESM is too repulsive in the original implementation. In addition, the repulsiveness depends on the width of the Gaussian charge as it should not because the Gaussian charge is introduced for a numerical reason.

We have found that in order to obtain the correct results, it is necessary to include all the terms for $V_{\text{loc}}^{\text{LR}}$ and $V_{\text{ion}}^{\text{LR}}$ resulting from the Green's functions not only for the vacuum, but also for the ESM regions. By the correct implementation, the results are no more dependent on the width of the fictitious Gaussian charges. We also found that overlap of the ion core and the ESM is allowed by modifying the short-range part of the ion-ion interaction energy ($E_{\text{ion}}^{\text{SR}}$). This lifts the limitation of the original ESM, enhancing the robustness and flexibility of the ESM method.

We have introduced the correct implementation of the smooth ESM into the QUANTUM-ESPRESSO [1] package and recalculated the total energy curves for the carbon monoxide (CO) (Fig. 2) and the water (H₂O) molecules (Fig. 3). We used the ultrasoft pseudopotentials [2,3] and the plane-wave cutoffs of 30 and 400 Ry for the wave functions and the augmentation charge, respectively.

For the calculations of CO, we used a $0.5 \times 0.5 \times 2.8 \text{ nm}^3$ unit cell, which is longer in the z direction than the one used in the original paper, and for H₂O, the same unit cell was used as in the original paper. The corrected figures for CO (Fig. 2) and H₂O (Fig. 3) are shown below. It is found that the smoothness parameter a should be much smaller than that presented in the original paper. We have found that in the vacuum region, the total energy decreases as the distance between the molecule and the ESM decreases, i.e., the interaction between the molecule and the ESM is attractive, whereas once the molecule penetrates into the ESM, the interaction becomes repulsive because of the screening of the potential by the ESM. Thus, the minimum of the total energy is located near the boundary between the vacuum and the ESM regions (z_1). Here, it should be noted that the total energy curve is not smooth at $z = z_1$ because the first derivative of the model permittivity is not continuous. Furthermore, when the z component of the atomic coordinate is located exactly at z_1 , special treatment for the $V_{\text{ion}}^{\text{SR}}$ is required. Thus, in a practical calculation, we suggest using a repulsive potential to prevent such a situation. Nevertheless, the overlap of the electron density with the ESM is allowed, and the advantage of the smooth ESM is not impaired.

FIG. 2. Total energy as a function of the longitudinal position of the CO molecule z_O and for different values of the smoothness parameter a .

FIG. 3. Total energy as a function of the longitudinal position of the water molecule and for different molecular orientations. $a = 0.0378 \text{ nm}^{-1}$ is used.

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