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**Improved modeling of electrified interfaces using the effective screening medium method** IKUTARO HAMADA, National Institute for Materials Science, OSAMU SUGINO, University of Tokyo, NICÉPHORE BONNET, University of Tokyo and National Institute of Advanced Industrial Science and Technology, MINORU OTANI, National Institute of Advanced Industrial Science and Technology — The effective screening medium (ESM) method has been developed as a way to simulate electrified interfaces within a first principles framework using periodic boundary conditions. Given a slab geometry standing for the interface, the ESM method allows filling the region away from the slab with a dielectric screening medium— the ESM per se—as a simple way to include electrostatic screening effect of the environment. In the original version of the ESM method, the relative permittivity changes discontinuously from  $\epsilon = 1$  to  $\epsilon > 1$  at the boundary located between the molecular system and the ESM, which causes numerical instability when the electron density of the molecular system touches the boundary. Here we improve upon the description of the screening medium by imposing a smooth transition of the dielectric permittivity between the molecular system and the ESM (smooth ESM), thus precluding numerical instabilities when molecules come in contact with the ESM. Moreover, at short distances, the smooth ESM acts as a repulsive wall, and thus the simulation cell can serve as a natural container for molecules in molecular dynamics simulations. Consequently, the smooth ESM method is a substantial advancement in modeling solid-liquid interfaces under electric bias.

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