A new approach to first principles calculation of charged surface/interface

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In surface science, because of computational efficiency and tractability, first principles calculations often use the slab model in which layers of atoms and a vacuum region are periodically repeated. Due to the periodic boundary condition (PBC), the slab model is well-known to have the difficulty in handling charged or polarized surfaces, and these surfaces have been, in an ad hoc manner, manipulated by introducing a compensating charge or dipole layer somewhere in the supercell. As a method of resolving this problem, we present here a new method, effective screening medium (ESM) method [1], which is systematic and widely applicable, but is reasonably simple and efficient.

The characteristic of our method is that a slab model, which is periodic in *x*- and *y*- directions, is located into semi-infinite vacua or effective media. The effective medium is only characterized by relative permittivity constant ε_r. If ε_r is infinity the effective medium stands for vacuum and if ε_r is a certain finite number, for example 78, the effective medium stands for water. We can model several physical situations by changing the permittivity constant and the boundary condition of the Poisson equation in *z*-direction. In these cases, the Poisson equation can be handled easily because it is quasi one-dimensional in *z*-direction, while the Kohn-Sham equation can be handled using supercell of finite length in *z*-direction because the electrons are localized within the atomic layer.

In our scheme, total-energy and atomic forces can be calculated without major increase of the computational cost, and is suitable for determining structure and conducting molecular dynamics. We will present several calculations to show availability of the method.

[1] M. Otani and O. Sugino, *Phys. Rev. B* (2006) **73**, 115407.