

Abstract Submitted
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A method for biased surface electronic structure: a planewave non-repeated slab approach MINORU OTANI, OSAMU SUGINO, Institute for Solid State Physics, Tokyo University — We have developed a new formalism for calculating electronic structures in a symmetric/asymmetric slab model [1]. The method can treat not only surfaces exposed to vacuum but also biased surfaces. To solve the Kohn-Sham equation, we adopt a conventional Kohn-Sham solver in a repeated slab model. On the other hand, for the Poisson equation, we solve it in a whole space along surface normal direction. Owing to this treatment we can easily obtain work functions of the surface and we can calculate polarized surfaces without dipole correction. By introducing an effective screening medium and imposing appropriate boundary conditions to the Poisson equation, we can calculate a surface that is placed in front of electrode. In this model it is possible to apply a bias voltage to the surface by changing the Fermi energy of the surface. Thus we can calculate electronic and geometric structures of the biased surface. This model corresponds to the experimental setup for the scanning tunneling microscopy or back-gate field effect transistor. The important advantage of the method is that we can easily implement it in a conventional first-principles calculation method. References: [1] M. Otani and O. Sugino, submitted to PRB.

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