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A multi-scale approach to the electronic structure of doped semiconductor surfaces OFER SINAI, Weizmann Institute of Science, Rehovoth, IL, OLIVER T. HOFMANN, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE, PATRICK RINKE, Aalto University School of Science, Aalto, FI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE, GEORG HEIMEL, Humboldt-Universität zu Berlin, Berlin, DE, LEEOR KRONIK, Weizmann Institute of Science, Rehovoth, IL — The inclusion of the global effects of semiconductor doping poses a unique challenge for first-principles simulations, because the typically low concentration of dopants renders an explicit treatment intractable. Furthermore, the width of the space-charge region (SCR) at charged surfaces often exceeds realistic supercell dimensions. We present a multi-scale technique that addresses these difficulties. It is based on the introduction of excess charge, mimicking free charge carriers from the SCR, along with a fixed sheet of counter-charge mimicking the SCR-related field. Self-consistency is obtained by imposing charge conservation and Fermi level equilibration between the bulk, treated semi-classically, and the electronic states of the slab/surface, which are treated quantum-mechanically. The method, called CREST - the Charge-Reservoir Electrostatic Sheet Technique - can be used with standard electronic structure codes. We validate CREST using a simple tight-binding model, which allows for comparison of its results with calculations encompassing the full SCR explicitly. We then employ it with density functional theory, obtaining insight into the doping dependence of the electronic structures of the metallic clean-cleaved Si(111) surface and its semiconducting (2x1) reconstructions.

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