

Abstract Submitted
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Optimal first-principles evaluation of electrostatic potentials: applications to interfacial band alignment and charged defect energies in bulk, surfaces and 2D materials YUAN PING, Department of Chemistry and Biochemistry, University of California, Santa Cruz, RAVISHANKAR SUNDARARAMAN, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180 — First-principles calculations of band alignment and charged defect formation energies require comparing electrostatic potential of different atomic configurations, which is made challenging by the strong oscillation of this potential at the atomic scale. We introduce a method to suppress these strong oscillations by eliminating the deep wells in the potential at each atom. We demonstrate that this method considerably improves the system-size convergence of a wide range of first-principles predictions that depend on alignment of electrostatic potentials, including band offsets at solid-liquid interfaces, and formation energies of charged defects in solids and at solid surfaces in vacuum and solution. In the end we show that our new approach of computing the charged defects significantly improved the supercell convergence for charged defects in 2D materials, which has been a long-standing problem in the field.

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