Abstract Submitted
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High Performance Computing for Large Systems: Using Real Space Pseudopotentials for Metal-Semiconductor Interfaces[1] JAIME SOUTO, JAMES R. CHELIKOWSKY, University of Texas at Austin, TZU-LIANG CHAN, Hong Kong Baptist University, KAI-MING HO, Iowa State University, CAI-ZHUANG WANG, Ames Laboratory, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — Solving for the electronic structure at an interface can be computationally intensive. Even at the interface between crystalline systems, the structural details may not be known. Mismatch between the crystalline systems can result in unit cells containing hundreds, if not thousands of atoms. Until recently, such systems were not computationally tractable. Real-space pseudopotential density functional theory has proven to be an efficient avenue for computing the properties of such systems. Fully self-consistent solutions have been routinely obtained for systems with thousands of atoms. We illustrate this method applied to a Pb(111)/Si (111) interface and in particular examine the evolution of a Schottky barrier for this interface. We examine systems up to 1,500 atoms and determine the details of how quantum confinement controls the electronic structure of this system.

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