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Quantum confined Schottky barriers: Tuning the Schottky-Mott and Bardeen Limits JAMES CHELIKOWSKY, TZU-LIANG CHAN, University of Texas at Austin, KAI-MING HO, Iowa State University and Ames Laboratory, CAI-ZHUANG WANG, Ames Laboratory, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — Even though metal-semiconductor junctions are an essential component in electronic devices, an atomistic understanding of the electronic structure of such junctions has remained elusive. Hundreds, if not thousands, of atoms may be required to model such interfaces, owing to lattice mismatches at the interface. The absence of a detailed understanding of the interface structure has inhibited the application of electronic structure calculations to examine the evolution of Fermi level pinning. Here we capitalize on recent computational breakthroughs and apply them to a prototypical system: a Pb(111) film on a Si(111) substrate. We consider up to 1,500 atoms in our first principle calculations based on real space pseudopotentials, and explicitly model the atomistic details of the metal-semiconductor interface. We propose a pinning mechanism for the Fermi level that depends critically on the role of quantum confinement in the overlaying metallic film. By changing the thickness of the overlying film, the pinning mechanism can be tuned from the abrupt interface description of Schottky and Mott to the metal induced gap state description of Bardeen.

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