First-Principles Theory for Schottky Barrier Physics

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The physics of Schottky contact is one of the most important topics in semiconductor physics. The macroscopic size of a Schottky barrier makes its modeling from firstprinciples a prohibitively difficult task. The physics of Schottky barrier is rich and has far-reaching impacts. The Schottky barrier depends on many factors, for example, the quality and structure of a semiconductor surface. A major contribution to the charge distribution near the interface is that from the metal induced gap states (MIGS). We develop a first-principles description of the physics of Schottky barrier, defining the induced charge in the bulk of semiconductor due to MIGS and electrostatic potential due to dipoles at the interface. Our method based on density functional theory and consists of calculation of evanescent states in the gap of the semiconductor based on complex band structure of the semiconductor surface, following by calculation of the induced charge in the bulk of semiconductor. The SBH is determined from the selfconsistency between the electrostatic potential and the induced charges in the bulk.

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