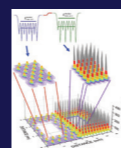


The Schottky barrier height (SBH) of a metal-semiconductor interface and the band offset (BO) of a semiconductor heterojunction interface are crucial to the performance of advanced solid-state devices and have been extensively investigated for decades. These interface parameters are direct results of and should be explained with interface charge distribution. For a long time, however, such a scientifically based approach was not possible and the explanation of SBH/BO largely fell into the hands of empirical models. There were several breakthroughs in this field in recent years that finally provided a scientific explanation of these band alignment conditions through charge distribution. In order to accomplish this, the long tradition of employing surface quantities to represent the solid crystals, dating back to the time of Schottky and Mott and followed by researchers ever since, was abandoned. Instead, “model solids” without surface dipoles were used as the proper representatives of solid crystals. This book discusses these recent developments, beginning with a semiclassical host-bath approach to analyze all energy-level-alignment problems. How the nearsightedness principle is used to construct model solids by neutral polyhedra theory (NPT) and to quantitatively model the SBH/BO with bulk crystal density is also explained in detail. The wide success of this density-based approach in the explanation/prediction of the BO at covalent, ionic, and polycrystalline heterojunction interfaces and the SBH at epitaxial and polycrystalline metal semiconductor interfaces is also examined. The “Fermi level pinning” phenomenon, which dominated the SBH/BO field and puzzled researchers for decades, also has a simple explanation from charge distribution, after the important issues of metallicity boundary and SBH inhomogeneity are recognized.

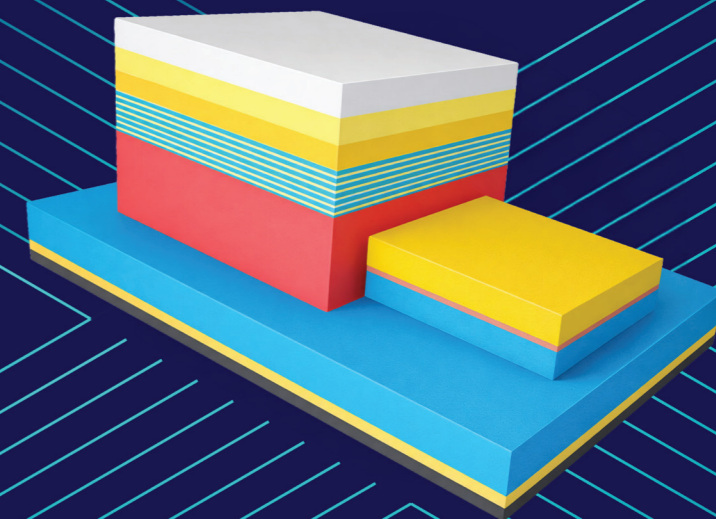
ENERGY LEVEL ALIGNMENT OF SOLID INTERFACES



Raymond T Tung

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