**Intermediate-phase Method for Computing the Natural Band Offset between Two Materials with Dissimilar Structures**

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**ABSTRACT**

The band offset between different semiconductors is an important physical quantity determining carrier transport properties near the interface in heterostructure devices. Computation of the natural band offset is a longstanding challenge. We propose an intermediate-phase method to predict the natural band offset between two structures with different symmetry, for which the superlattice model cannot be directly constructed. With this method, and the intermediate phases obtained by our searching algorithm, we successfully calculate the natural band offsets for two representative systems, (i) zinc-blende CdTe and wurtzite CdS and (ii) diamond and graphite. The calculation shows that the valence band maximum (VBM) of zinc-blende CdTe lies 0.71 eV above that of wurtzite CdS, close to the result 0.76 eV obtained by the three-step method. For the natural band offset between diamond and graphite which could not be computed reliably with any superlattice methods, our calculation shows that the Fermi level of graphite lies 1.51 eV above the VBM of diamond using a newly identified intermediate phase. This method, under the assumption that the transitivity rule is valid,can be used to calculate the band offsets between any semiconductors with different symmetry on condition that the intermediate phase is reasonably designed.[1]

[1] H. J. Gu, Y. Y. Zhang, S. Y. Chen, H. J. Xiang, and X. G. Gong, Phys. Rev. B **97**, 235308 (2018)

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