MAR14-2013-020044

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Band alignment of zinc-blende and chalcopyrite semiconductors: Effects of misfit dislocations

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The band offset is a key quantity that largely determines electrical transport across the heterointerfaces in electronic devices and photovoltaic cells. Its accurate determination has therefore been one of the central issues in computational materials science. The band offset by nature depends on the atomistic and electronic structure of heterointerfaces. Assuming such dependences to be weak at interfaces composed of structurally and chemically similar materials, a band alignment diagram, where relevant materials are aligned using a common reference level, carries information of the band offsets. Quantities such as branch points from bulk calculations and ionization potentials from surface calculations, as well as band offsets explicitly obtained from interface calculations, have been used for the alignment, but the effects of misfit dislocations at semicoherent interfaces have been neglected. In this talk I will revisit the band alignment of zinc-blende and chalcopyrite semiconductors using semilocal and hybrid density functional calculations [1-4]. In particular, the effects of misfit dislocations on the band offsets are discussed for selected zinc-blende heterointerfaces via explicitly treating edge dislocation arrays in the calculations [1]. The variation in the electrostatic potential associated with the presence of misfit dislocations is found to be localized around the dislocation cores. The misfit dislocations typically affect the band offsets by only about 0.1 eV at a distance of 1 nm from the interfaces.

[1] Y. Hinuma, F. Oba, and I. Tanaka, Phys. Rev. B 88, 075319 (2013).
[2] Y. Hinuma, F. Oba, Y. Kumagai, and I. Tanaka, Phys. Rev. B 88, 035305 (2013).
[3] Y. Hinuma, F. Oba, Y. Nose, and I. Tanaka, J. Appl. Phys. 114, 043718 (2013).
[4] Y. Hinuma, F. Oba, Y. Kumagai, and I. Tanaka, Phys. Rev. B 86, 245433 (2012).