Materials Science and Technology Division
Materials Theory Group

"A Look at the Electronic Structure of Semiconducting Alloys using a Hybrid Screened Functional"

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Abstract

Semiconducting alloys make up just about every optoelectronic device in use today through their ability to tune band gaps. These alloys have such great importance in the optoelectronic engineering community that many optoelectronic growers refer to their band gap vs lattice constant plot as the "map of the world". The screened hybrid functional, HSE06, used in density functional theory (DFT) has been gaining traction recently for its predictive powers of the band structure in bulk semiconductors. It is natural to assume that these accurate results would carry over to the more relevant alloy semiconductors, but little work has been done to confirm this. We investigate the compositional dependence on the electronic structure for a range of III-V semiconducting alloys as well as the HgCdTe alloy. The former exhibit a critical composition where the band gap crosses over from a direct band gap to an indirect band gap, whereas the latter exhibit a semimetal to semiconductor crossover. We also investigate the quality of HSE06 when predicting band alignment in such alloy heterostructures. A direct comparison is made between the HSE06 functional and the commonly used PBE standard density functional with experiment, revealing that HSE06 is by far the more reliable functional for tuning the electronic properties of semiconducting alloys.

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