Hybrid Density Functional Study of the Electronic Properties for (Hg,Cd)Te Systems

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The HgCdTe alloy is used in high-performance infrared detection applications with a band gap range extending across the infrared spectrum. HgTe in particular has sparked interest for its topological insulating behavior in quantum well devices due to its band inverted nature. We test the quality of the newer hybrid screened functional, HSE, on the two contrasting materials: HgTe (semimetal) and CdTe (semiconductor) to see how well it performs under a range of setupsi [1]. A direct comparison of HSE with the standard DFT functional PBE to experiment for the HgCdTe alloy reveals HSE is able to reproduce the experimental crossover composition of 17% Cd concentration when the alloy goes from a semimetal to semiconductor, whereas PBE overestimates this composition at 67% Cd concentration. HSE also predicts a higher valence band offset of 0.53 eV in the HgTe/CdTe heterostructure than previous first-principle and early experimental results, but in good agreement with the more recent experimental results.

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[1] J. W. Nicklas and J. W. Wilkins, Phys. Rev. B **84**, 121308(R) (2011).

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