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Predicting the Direct to Indirect Transition in III-V Alloys JEREMY NICKLAS, JOHN WILKINS, The Ohio State University — The screened hybrid functional, HSE, 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 alloy semiconductors, but little work has been done to confirm this. We recently investigated the compositional dependence on the electronic band structure for a range of III-V semiconducting alloys (AlGaAs, InAlAs, AlInP, InGaP, and GaAsP) [1]. These alloys have a critical composition where the band gap crosses over from a direct band gap (having optoelectronic uses) to an indirect band gap (window layers in solar cells). A direct comparison of this critical composition is made between HSE and the standard density functional, PBE, revealing crossover compositions within 12% atomic composition when compared to experiment while PBE overestimates by as much as 39% atomic composition. Such results give merit that HSE is a reliable functional for tuning the electronic properties of semiconducting alloys.

[1] Jeremy W. Nicklas and John W. Wilkins, Appl. Phys. Lett. 97, 091902 (2010)

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