

Abstract Submitted  
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**Hybrid DFT computes accurate band offsets of semiconductor alloy heterostructures**<sup>1</sup> AMITA WADEHRA, JEREMY NICKLAS, JOHN WILKINS, The Ohio State University — Semiconductor alloy heterostructures are the backbone of optoelectronic devices. Among the most important parameters that determine the utility of heterostructure devices are the valence and conduction band offsets. Although DFT with standard functionals such as LDA or PBE does an acceptable job for valence band offsets, it fails to predict accurate conduction band offsets on its own due to the well-known band gap problem. We demonstrate the accuracy of HSE (Heyd-Scuseria-Ernzerhof) hybrid functional for computing the band gaps and band offsets of a broad selection of technologically important semiconductor alloys and their heterostructures, e.g., AlInAs/GaInAs, GaInP/AlGaAs, AlInP/GaInP [1]. The highlight of this study is the computation of conduction band offsets with a reliability that has eluded standard density functional theory. These results demonstrate predictive power of HSE for band engineering of relevant devices.

[1]. A. Wadehra, J. W. Nicklas and J. W. Wilkins, Appl. Phys. Lett. 97, 092119 (2010)

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Amita Wadehra  
The Ohio State University

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