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Band-offsets of semiconductor heterostructures using hybrid density functionals[1] AMITA WADEHRA, JOHN W. WILKINS, Ohio State University, RICHARD G. HENNIG, Cornell University, GUSTAVO E. SCUSERIA, Rice University — The performance of novel devices, e.g., HEMTs based on semiconductor heterostructures, depend strongly on their conduction and valence band-offsets. However, conventional density functional theory based on LDA and GGA fails for narrow-gap semiconductors such as InAs, predicting it to be a metal. An accurate treatment of such systems requires self-consistent DFT calculations with hybrid functionals such as B3LYP and HSE. B3LYP success for a wide variety of atoms and molecules is computationally challenging to translate to solids. We compare band gaps and band offsets of strained and unstrained InAs/InP and InAs/AlAs heterostructures calculated with these hybrid functionals. Our preliminary results agree well with experimental and other theoretical investigations.

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