

Abstract Submitted
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Band offsets of semiconductor heterostructures : dependence on density functionals¹ AMITA WADEHRA, RICHARD G. HENNIG, JOHN W. WILKINS, Department of Physics, Ohio State University, Columbus, OH 43210, GUSTAVO E. SCUSERIA, Department of Chemistry, Rice University, Houston, TX 77005 — There is an increasing interest in In-based heterostructures for HEMT. Predictions of band offsets could speed up the development process of these devices. We assess various exchange-correlation potentials including hybrid functionals such as HSE ² to analyze electronic properties and structural energetics of such systems. We calculate the band gaps and band offsets of InAs heterostructures such as InAs/InAlAs and InAs/InAsP. We also show a comparison of the structural energies for interfaces and site substitutions obtained by using different functionals. An accurate estimation of these properties is crucial for their application in the manufacture and performance of novel semiconductor devices.

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²J. Heyd, J.E. Peralta, G.E. Scuseria and R.L. Martin, *J. Chem. Phys.* **123**, 174101 (2005).

Amita Wadehra
Department of Physics, Ohio State University, Columbus, OH 43210

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