

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**B3LYP Works for Semiconductors Heterostructures** JEREMY NICKLAS, JOHN WILKINS, Ohio State University — The B3LYP functional with Gaussian basis functions gives reliable valence band offsets (VBO) of heterostructures involving, for example, GaN, AlN, and InN. The density of states of the inner bulk layers in the heterostructure estimates the valence band offset while confirming the bulk bandgaps. The VBO is calculated for the cubic and hexagonal structures with a range of lattice constants. For example, cubic-AlN and cubic-GaN heterostructure with 8+8 (001) layers show decreasing VBO with increasing (001) planar lattice: 0.98 eV for 4.38 Å, 0.97 eV for 4.45 Å, and 0.85 eV for 4.52 Å. These are consistent with previous GWA calculations [1]. [1] D. Cociorva, W. G. Aulbur and J. W. Wilkins, Solid State Communications 124, 63-66 (2002).

Jeremy Nicklas  
Ohio State University

Date submitted: 19 Nov 2006

Electronic form version 1.4