Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

The density functional theory defect band gap in GaAs[1] PETER A. SCHULTZ, Sandia National Laboratories — Using a total energy method with detailed control of electrostatic boundary conditions, esp. the chemical potential for net charge, the computed charge transition levels of simple intrinsic defects in GaAs within density functional theory are presented. The levels are demonstrated to be converged with supercell size, and largely insensitive to the functionals and pseudopotentials used. The results accurately reproduce available experimental data. The range of defect levels, a defect band gap, spans a full experimental band gap regardless of the size of the Kohn-Sham gap of the underlying functional-pseudopotential context used. The defect band gap, based on extrapolated total energy differences, is a better predictor of the fundamental gap than the Kohn-Sham eigenvalue gap. Based on the quantitative predictions of the levels, these results lead to a reassessment of long-standing defect assignments in GaAs, reconciling seemingly contradictory observations.

[1]Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Date submitted: 19 Nov 2009 Electronic form version 1.4