

Defect levels in semiconductors: Is the "band gap problem" truly a problem?

Peter A. Schultz

*Multiscale Computational Materials Methods, Sandia National Laboratories
Albuquerque, NM 87185, USA*

Predictive calculations of defect levels in semiconductors using density functional theory (DFT) have been crippled by two issues: the supercell approximation, which invokes boundary conditions inconsistent with an isolated defect, and the band gap problem, where DFT calculations are seen to significantly underestimate the fundamental band gap. The DFT gap in silicon, for example, is less than half the experimental band gap. Since the band gap defines the interesting energy scale for defect levels, this would appear to preclude quantitative predictions. I present a method that addresses the deficiencies of the standard supercell approximation and constitutes a more rigorous, internally consistent computational model for an isolated defect. This model incorporates electrostatic boundary conditions appropriate to an isolated charged defect, identifies a common electron reservoir for the net charge of all defects, deals explicitly with defect banding, and incorporates bulk polarization. The new methodology is applied to an extended suite of defects in silicon. The resulting defect energy level spectrum spans the experimental band gap, i.e., exhibits no band gap problem, and agrees remarkably well with experiment.

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