

Abstract Submitted
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Defect levels in semiconductors - is the band gap problem truly a problem?¹ PETER A. SCHULTZ, Sandia National Laboratories, Albuquerque, NM — Quantitative predictions of defect properties in semiconductors using density functional theory (DFT) have been crippled by standard supercell methods, which have incorrect boundary conditions for an isolated defect, and the band gap problem, where DFT drastically underestimates the band gap. I present a generalized supercell method with boundary conditions appropriate to point defects, to fix the electrostatic boundary conditions, remove ambiguity in charge reservoir, include bulk polarization effects, and specifically account for defect level dispersion. I compute formation energies for an extensive set of defects in silicon. The resulting defect level spectrum in silicon exhibits no band gap problem. The results agree remarkably well with experiment for those values that are experimentally known, and predict heretofore unobserved electronic transitions important for the electrical response of irradiated semiconductor devices.

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