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First-principles simulations of GaAs defects: The challenge of Ga pseudopotentials PETER A. SCHULTZ, O. ANATOLE VON LILIENFELD, Sandia National Laboratories, Albuquerque, NM — Design of norm-conserving gallium pseudopotentials (PP) has been investigated for density functional theory calculations of defects in GaAs. A converged PP construction is described. We examined the performance in cubic zinc-blende structure phases of GaAs, GaP, and GaN. Computed lattice constants, bulk moduli, and, particularly, band gaps vary greatly depending on PP construction and exchange correlation functional. The Kohn Sham band gaps exhibit a distinctive sensitivity on lattice constant, direct with a strong near-linear dependence at larger lattice constants with crossover to indirect near (within 5%) of the equilibrium lattice constant. Gradient-corrected functionals with a converged PP give a near-zero GaAs gap, a problem for defect calculations. A 3d-core PP "fixes" the band gap, but predicts GaAs defect formation energies different from converged 3d-valence PP. 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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