

Abstract Submitted
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Simple intrinsic defects in GaP and InP PETER A. SCHULTZ, Sandia National Laboratories, Albuquerque, NM — To faithfully simulate evolution of defect chemistry and electrical response in irradiated semiconductor devices requires accurate defect reaction energies and energy levels. In III-Vs, good data is scarce, theory hampered by band gap and supercell problems. I apply density functional theory (DFT) to intrinsic defects in GaP and InP, predicting stable charge states, ground state configurations, defect energy levels, and identifying mobile species. The SeqQuest calculations incorporate rigorous charge boundary conditions removing supercell artifacts, demonstrated converged to the infinite limit. Computed defect levels are not limited by a band gap problem, despite Kohn-Sham gaps much smaller than the experimental gap. As in GaAs, [P.A. Schultz and O.A. von Lilienfeld, Modeling Simul. Mater. Sci. Eng. 17, 084007 (2009)], defects in GaP and InP exhibit great complexity—multitudes of charge states, bistabilities, and negative U systems—but show similarities to each other (and to GaAs). Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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