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Discriminating a deep defect from shallow acceptors in supercell calculations: gallium antisite in GaAs PETER SCHULTZ, Sandia National Laboratories — To make reliable first principles predictions of defect energies in semiconductors, it is crucial to discriminate between effective-mass-like defects—for which existing supercell methods fail—and deep defects—for which density functional theory calculations can yield reliable predictions of defect energy levels. The gallium antisite Ga_{As} is often associated with the 78/203 meV shallow double acceptor in Ga-rich gallium arsenide. Within a framework of level occupation patterns, analyses of structure and spin stabilization can be used within a supercell approach to distinguish localized deep defect states from shallow acceptors such as B_{As}. This systematic analysis determines that the gallium antisite is inconsistent with a shallow state, and cannot be the 78/203 shallow double acceptor. The properties of the Ga antisite in GaAs are described, predicting that the Ga antisite is a deep double acceptor and has two donor states, one of which might be accidentally shallow. — 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 Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

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