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Density functional calculations of point defects in InAs[1]
JONATHAN MOUSSA, PETER SCHULTZ, Sandia National Laboratories — Standard semilocal density functionals do not generate a gap in the Kohn-Sham eigenvalues for InAs, a semiconductor with an experimental gap of 0.4 eV. Without a theoretical band gap, it becomes difficult to identify, specify, and characterize pure localized states of point defects with energy levels within the experimental band gap. The bulk band gap problem can be alleviated with screened hybrid density functionals, such as the Heyd-Scuseria-Ernzerhof (HSE) functional, that open the generalized Kohn-Sham eigenvalue gap of InAs to near the experimental value. However, even without a Kohn-Sham gap, the local moment countercharge (LMCC) method [Phys. Rev. Lett. 96, 246401 (2006)] is able to predict charge transition energy levels of localized defect states, using standard semi-local functionals. We present an LMCC-based study of standard point defects in InAs using semilocal density functionals and compare the results to HSE-based calculations to assess the validity of LMCC calculations in this situation.

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