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Surface effects in Si interstitial formation energies ANN E. MATTSSON, RYAN R. WIXOM, Sandia National Laboratories, Albuquerque, NM, RICKARD ARMIENTO, University of Bayreuth, Germany — We are calculating Si self-interstitial formation energies using Density Functional Theory and several different exchange-correlation energy functionals. We show that the difference in results obtained with the LDA, PBE, PW91, and AM05 [1] functionals can be explained by the functionals' different surface intrinsic errors. We explain why surface effects are important for formation energies of interstitials in semi-conductors. Surface effects have previously been studied for metal vacancy formation energies. 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. [1] R. Armiento and A. E. Mattsson, Phys. Rev. B **72**, 085108 (2005).

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