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Density Functional Theory Calculations of Activation Energies for Carrier Capture by Defects in Semiconductors N. A. MODINE, A. F. WRIGHT, S. R. LEE, Sandia National Laboratories — The rate of defect-induced carrier recombination is determined by both defect levels and carrier capture cross-sections. Density functional theory (DFT) has been widely and successfully used to predict defect levels, but only recently has work begun to focus on using DFT to determine carrier capture cross-sections. Lang and Henry developed the theory of carrier-capture by multiphonon emission in the 1970s and showed that carrier-capture cross-sections differ between defects primarily due to differences in their carrier capture activation energies. We present an approach to using DFT to calculate carrier capture activation energies that does not depend on an assumed configuration coordinate and that fully accounts for anharmonic effects, which can substantially modify carrier activation energies. We demonstrate our approach for intrinsic defects in GaAs and GaN and discuss how our results depend on the choice of exchange-correlation functional and the treatment of spin polarization. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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