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Density Functional Theory Calculations of Activation Energies for Carrier Capture by Defects in Semiconductors NORMAND MODINE, ALAN WRIGHT, STEPHEN LEE, Sandia National Laboratories — Carrier recombination due to defects can have a major impact on device performance. The rate of defect-induced 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 worked out the fundamental theory of carrier-capture by multiphonon emission in the 1970s and showed that, above the Debye temperature, 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 the -3/-2 level of the Ga vacancy in wurtzite GaN. 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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