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Quantum Monte Carlo calculation of point defect thermal and optical ionization levels: application to magnesium oxide and zinc oxide
ELIF ERTEKIN, LUCAS WAGNER, University of Illinois, JEFFREY GROSSMAN, Massachusetts Institute of Technology — From electronics to optoelectronics to photovoltaics, point defects influence and dominate the properties of semiconducting materials. Quantitative descriptions of the effect of point defects on electronic, optical, and transport properties are critical to enabling point-defect engineering for materials design. However, accurate prediction of point-defect energetics, thermal ionization energies, and optical transition energies from first principles remains a challenge. We present an approach to calculation of point defect optical and thermal ionization energies based on the highly accurate quantum Monte Carlo methods, and demonstrate it for the oxygen vacancy in the binary ionic compound magnesium oxide and the substitutional nitrogen impurity in zinc oxide. The use of quantum Monte Carlo, an inherently many–body theory that directly treats electron correlation, offers many improvements: it can help overcome the band gap problem in density functional theory and obviate the need for ad-hoc corrections. Our computed optical and thermal ionization energies are in excellent agreement with experimental and/or other high-accuracy results.

Elif Ertekin
University of Illinois

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