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Identification of polaronic defects in wide band gap semiconductors via diffusion Monte Carlo JAEHYUNG YU, ELIF ERTEKIN, Univ of Illinois - Urbana — Polaronic defects are important to understanding a wide variety of properties in semiconductors; for instance they are closely coupled to electron phonon interactions and can greatly affect carrier concentrations and mobilities. The formation of a polaronic defect in a semiconductor is an interesting phenomenon because it incorporates a trade off between electron localization and structural relaxation. Because of its small energy scale and the localized nature of polaronic defect levels, accurately describing polaronic defects in semiconductors requires high accuracy first principle calculation methods. We demonstrate the use of the fixed node diffusion Monte Carlo (DMC) method to the identification of polaronic nitrogen defects in the wide band gap semiconductor zinc oxide. Using DMC, we can demonstrate that nitrogen defects in ZnO are subject to a symmetry-breaking Jahn-Teller distortion, which deepens the defect level in the band gap. Our DMC results for defect transition levels and optical transitions are in good agreement with recent experiments. Our results demonstrates that highly accurate treatment of electron correlation can improve predicition of defect properties in challenging semiconductor materials.

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