Quantum Monte Carlo calculations of defects in ZnO

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The semiconductor ZnO holds much promise for many applications due to its ability to display a wide variety of properties. However, an understanding of the structure and electronic structure of the defects which lead to the material's properties has proven difficult. Previous density functional theory (DFT) calculations by Van De Walle et. al. [1] using the local density approximation, suggest that hydrogen interstitials and oxygen vacancies may be the dominant defect present in the as-grown material leading to its n-type conductivity. However, the corrections accounting for DFT's band gap problem lead to a wide variance in defect formation energies reported and uncertainty in the qualitative results. More recent calculations such as those by Oba et. al. [2] using the HSE hybrid functional confirm the presence of these defect structures and their electronic transition levels. However, the results of various DFT studies lack the level of quantitative agreement necessary for successful device engineering. We are performing Quantum Monte Carlo calculations for the defects in ZnO to determine the defect formation energies and transition levels as well as to verify the previous DFT calculations and evaluate different DFT methodologies.

[1] C. G. van de Walle, Phys. Rev. Lett. 85, 1012 (2000).

[2] F. Oba, Phys. Rev. B 77, 245202 (2008).