Quantum Monte Carlo methods for accurate treatment of the bulk and defect properties of semiconductors

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Obtaining accurate descriptions of the bulk and defect properties of semiconductors from first principles remains a challenge, particularly for wide gap materials and oxides. In spite of many recent developments and improvements to the degree of accuracy attainable, there remain several challenges to overcome before our methods are truly quantitative and predictive. To this end, recently we have been exploring the application of the fixed node diffusion Monte Carlo method to obtaining high-accuracy descriptions of the bulk and point-defect properties of semiconductors, focusing on historically challenging systems. The question we wish to answer is; "how well can we do using this approach, and how does it compare to other methods?" I will present some examples from our recent work, which include phase stability in antiferromagnetic manganese oxide polymorphs, ground and excited state properties of zinc oxide and zinc selenide, and nitrogen point defects in zinc oxide. In general, although there remain several challenges to overcome, the use of a many-body approach that directly treats electron correlation offers the possibility of high accuracy, systematically improvable descriptions. We find that in many cases where other methods struggle, the FN-DMC method gives quantitative results in good agreement with experiment and/or other high-accuracy treatments.