Quantum Monte Carlo calculations for point defects in semiconductors

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Point defects in silicon have been studied extensively for many years. Nevertheless the mechanism for self diffusion in Si is still debated. Direct experimental measurements of the selfdiffusion in silicon are complicated by the lack of suitable isotopes. Formation energies are either obtained from theory or indirectly through the analysis of dopant and metal diffusion experiments. Density functional calculations predict formation energies ranging from 3 to 5 eV depending on the approximations used for the exchange-correlation functional [1]. Analysis of dopant and metal diffusion experiments result in similar broad range of diffusion activation energies of 4.95 [2], 4.68 [3], 2.4 eV [4]. Assuming a migration energy barrier of 0.1-0.3 eV [5], the resulting experimental interstitial formation energies range from 2.1 - 4.9 eV. To answer the question of the formation energy of Si interstitials we resort to a many-body description of the wave functions using quantum Monte Carlo (QMC) techniques. Previous QMC calculations resulted in formation energies for the interstitials of around 5 eV [1,6]. We present a careful analysis of all the controlled and uncontrolled approximations that affect the defect formation energies in variational and diffusion Monte Carlo calculations. We find that more accurate trial wave functions for QMC using improved Jastrow expansions and most importantly a backflow transformation for the electron coordinates significantly improve the wave functions. Using zero-variance extrapolation, we predict interstitial formation energies in good agreement with hybrid DFT functionals [1] and recent GW calculations [7].

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