Silicon-interstitials-based benchmarking of DFT exchange-correlation potentials

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Diffusion Monte Carlo (DMC) benchmarks DFT functionals: LDA, GGA, and HSE [1]. Extensive DFT studies on single-, di-, and tri-interstitials [2] provide stable structures and converged energies. For single-interstitial formation energies, our DMC results confirm earlier work [3], with 1.5 and 1.0 eV underpredictions for LDA and GGA, respectively. We continue to observe this trend in most di- and tri-interstitials. Additionally, we find HSE reproduces DMC results for single-interstitals. Preliminary analysis indicates that large LDA and GGA discrepancies with DMC occur for highly distorted defect configurations. Supported by DOE(DE-FG02-99ER45795), NSF (EAR-0530301, DMR-0205328), and Sandia National Laboratory. Computation performed at OSC and NERSC.

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