Quantum Mechanical Predictions of Defect Properties for Realistic Device Simulations

K. P. Driver[1], W. D. Parker[1], R. G. Hennig[1], Y. A. Du[1], J. W. Wilkins[1], E. Batista[2], R. L. Martin[2], G. Scuseria[3], C. J. Umrigar[4]

[1]Ohio State University, Columbus, OH
[2]Los Alamos National Laboratory, Los Alamos, NM
[3]Rice University, Houston, TX, [4]Cornell University, Ithaca, NY

Silicon self-interstitial defects play a major role in the fabrication and production of silicon devices. Simulations complement experimental efforts to understand the formation and evolution of these defects. We discuss the importance of a multi-prong approach to the computational effort. Transition state methods are used to identify defect geometries and pathways. DFT-based methods refine the geometries and pathways. Ultimately, quantum Monte Carlo measures the accuracy of results. Extensive DFT studies on single-, di-, and tri-interstitials have identified point to extended defect evolution. Single interstitials precipitate small, compact defects, which grow into larger four-interstitial defects. Compact four-interstitial defects frustrate growth of extended structures, while chain four-interstitials nucleate extended defects [1]. Diffusion Monte Carlo (DMC) benchmarks DFT functionals: LDA, GGA, meta-GGA, and HSE [2]. LDA and GGA tend to underestimate single-interstitial formation energies by 1.5 and 1.0 eV [3], respectively, while HSE shows much better agreement with DMC.

[1] D. A. Richie, J. Kim, S. A. Barr, K. R. A. Hazzard, R. G. Hennig, and J. W. Wilkins. *Phys. Rev. Lett.* **92**, 45501 (2004).

[2] J. Heyd *et al.*, J.Chem.Phys. **118**, 8207 (2003).

[3] W. -K. Leung, R. J. Needs, G. Rajagopal, S. Itoh, and S. Ihara. *Phys. Rev. Lett.* **83**, 2351 (1999).