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Backflow transformation improves QMC calculations of silicon self-interstitial defects[1] WILLIAM D. PARKER, KEVIN P. DRIVER, JOHN W. WILKINS, Ohio State University, RICHARD G. HENNIG, Cornell University — Recent advances in quantum Monte Carlo (QMC) reduce error introduced by approximations. Direct improvement of the trial wave function through backflow transformation of the electron coordinates[1] produces a wave function closer to the ground state by moving electrons out of the way of a given electron. Adding plane waves of particle position to the Jastrow factor[2] augments the accounting for interparticle correlation in QMC calculations by capturing the "corners" of the simulation cell neglected when the Jastrow is only a function of pair separation. Hybrid density functionals have produced better starting trial wave functions for molecules by incorporating some exact exchange to more accurately describe electron-electron interactions. We apply backflow transformation, plane-wave-expanded Jastrow factors and hybrid functional trial wave functions to QMC calculations of silicon self-interstitial defects. [1] López-Ríos *et al.*, Phys. Rev. E **74**, 066701 (2006). [2] Drummond *et al.*, Phys. Rev. B **70**, 235119 (2004).

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William Parker
Ohio State University

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