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Quantum Monte Carlo Benchmarks Functionals for Silica Polymorphs K.P. DRIVER, J.W. WILKINS, Ohio State U., R.G. HENNIG, C.J. UMRIGAR, Cornell U., G. SCUSERIA, Rice U., B. MILITZER, R.E. COHEN, Carnegie Institution of Washington — For many silica polytypes, the local density approximation (LDA) does a better job than the generalized gradient approximation (GGA) in predicting structural properties and bulk moduli. However, gradient corrections to the charge density are necessary for accurate phase energy differences [1]. Functionals that go beyond GGA may improve the accuracy of both structures and energies. For example, a meta-GGA functional, TPSS, and hybrid functionals B3LYP and HSE [2] have shown improvement in other systems [3]. We compare results from these functionals for structural properties, energy differences, and bulk moduli for a few high pressure phases of silica, and benchmark the results with Quantum Monte Carlo (QMC). Preliminary QMC results indicate that careful wavefunction optimization and finite size effects are of particular importance in obtaining accurate silica phase properties. Supported by DOE(DE-FG02-99ER45795), NSF (EAR-0530301, DMR-0205328), and Sandia National Laboratory. Computation at OSC and NERSC.

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K. P. Driver
Ohio State U.

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