Quantum Monte Carlo Benchmarks Functionals for Silica Poly- 
morphs K.P. DRIVER, J.W. WILKINS, Ohio State U., R.G. HENNIG, C.J. UMRI- 
GAR, Cornell U., G. SCUSERIA, Rice U., B. MILITZER, R.E. COHEN, Carnegie 
Institution of Washington — For many silica polytypes, the local density approxima- 
tion (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 func- 
tionals 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.