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High-temperature high-pressure properties of silica from Quantum Monte Carlo and Density Functional Perturbation Theory R.E. COHEN, Geophysical Lab., Carnegie Institution, K. DRIVER, Ohio State University, Z. WU, B. MILITZER, University of California, Berkeley, P.L. RIOS, M. TOWLER, R. NEEDS, University of Cambridge — We have used diffusion quantum Monte Carlo (DMC) with the CASINO code with thermal free energies from phonons computed using density functional perturbation theory (DFPT) with the ABINIT code to obtain phase transition curves and thermal equations of state of silica phases under pressure. We obtain excellent agreement with experiments for the metastable phase transition from quartz to stishovite. The local density approximation (LDA) incorrectly gives stishovite as the ground state. The generalized gradient approximation (GGA) correctly gives quartz as the ground state, but does worse than LDA for the equations of state. DMC, variational quantum Monte Carlo (VMC), and DFT all give good results for the ferroelastic transition of stishovite to the $CaCl_2$ structure, and LDA or the WC exchange correlation potentials give good results within a given silica phase. The ΔV and ΔH from the $CaCl_2$ structure to α-PbO_2 is small, giving uncertainly in the theoretical transition pressure. It is interesting that DFT has trouble with silica transitions, although the electronic structures of silica are insulating, simple closed-shell with ionic/covalent bonding. It seems like the errors in DFT are from not precisely giving the ion sizes.

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