Quantum Monte Carlo Study of the Elastic Instability of Stishovite Under Pressure

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Stishovite is a octahedrally coordinated polymorph of silica which is stable at pressures within Earth's lower mantle (10 GPa). Elastic properties of stishovite are important for explaining seismic structure and it serves as a model system for other six-coordinated silicates. Near 50 GPa, stishovite transforms to the $CaCl_2$-type structure due to an instability in the elastic shear modulus. The instability was first predicted by density functional theory (DFT) calculations and later confirmed by Raman spectroscopy and X-ray diffraction. At a computational cost of several million of cpu hours, Quantum Monte Carlo accurately predicts elastic constants and benchmarks previous DFT results on the stishovite elastic instability. Over the pressure range of 0 to 50 GPa, QMC shows the elastic shear modulus softens from 270 to 0 GPa in agreement with previous DFT and experimental results. The success of QMC elasticity predictions provides new opportunities to constrain seismic mineral data on other minerals and further our understanding of Earth's interior. Computations were performed at NERSC on the Cray-XT4 within the early user program. Financial support is provided by the NSF (EAR-0530282, EAR-0310139) and the DOE (DE-FG02-99ER45795).