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Quantum Monte Carlo Study of Elastic Instability in Stishovite
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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. 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. Computations were performed at NERSC. Funding provided by the NSF (EAR-0530282, EAR-0310139) and the DOE (DE-FG02-99ER45795).

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