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Quantum Monte Carlo Simulations of the Quartz to Stishovite Transition in SiO_2[1] R.E. COHEN, Carnegie Institution of Washington, MIKE TOWLER, PABLO LOPEZ RIOS, NEIL DRUMMOND, RICHARD NEEDS, TCM, Cavendish Laboratory, University of Cambrigde, U.K — The quartz-stishovite transition has been a long standing problem for density functional theory (DFT). Although conventional DFT computations within the local density approximation (LDA) give reasonably good properties of silica phases individually, they do not give the energy difference between quartz and stishovite accurately. The LDA gives stishovite as a lower energy structure than quartz at zero pressure, which is incorrect. The generalized gradient approximation (GGA) has been shown to give the correct energy difference between quartz and stishovite (about 0.5 eV/formula unit) (Hamann, PRL 76, 660, 1996; Zupan et al., PRB 58, 11266, 1998), and it was generally thought that the GGA was simply a better approximation than the LDA. However, closer inspection shows that other properties are not better for the GGA than the LDA, so there is room for improvement. A new density functional that is an improvement for most materials unfortunately does not improve the quartz-stishovite transition (Wu and Cohen, PRB 73, 235116, 2006). We are performing QMC computations using the CASINO code to obtain the accurate energy difference between quartz and stishovite to obtain more accurate high pressure properties, and to better understand the errors on DFT and how DFT can be improved.

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