Hybrid Density Functional Performance for Silica

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Silica is the most abundant and simplest mineral influencing the geological processes inside Earth. The accuracy in which silica properties are predicted with density functional theory (DFT) is highly dependent on the approximate functional used. The local density approximation 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, such as hybrid B3LYP and HSE [2,3] functionals, may improve the accuracy of both structures and energies. We compare results from these functionals for structural properties, energy differences, and bulk moduli for the quartz-stishovite phase transition, and benchmark the energy differences with quantum Monte Carlo (QMC). Preliminary results indicate that B3LYP predicts both structural and energetic properties accurately. B3LYP can potentially be used to predict properties of less well known post-stishovite phases of the lower mantle and as input for QMC calculations of lower mantle minerals.

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