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Stability and lattice dynamics of SiO_2 cristobalite SINISA COH, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — Among the phases of SiO_2 are alpha and beta cristobalite. Despite early indications that the higher-temperature beta phase might be cubic ($Fd\bar{3}m$), it is now accepted that it is in fact tetragonal ($I\bar{4}2d$), and that the experiments suggesting a cubic structure were averaging spatially or dynamically over tetragonal domains. Recently, Zhang and Scott (J. Phys. Cond.Matt. **19**, 275201) suggested that the lower-temperature alpha phase, widely accepted to be tetragonal ($P4_12_12$), might be an artifact in a similar way. With this motivation we investigate the energy landscape in the vicinity of cristobalite phases using first-principles calculations. We use the ABINIT implementation of density-functional theory in a plane-wave pseudopotential framework. We find that both the $P4_12_12$ alpha and $I\bar{4}2d$ beta phases are local minima, thus reinforcing that the identification of the alpha phase as belonging to the $P4_12_12$ structure. We compute the frequencies of phonon modes at high-symmetry k-points in both structures and compare with experiment. We also identify a minimum-energy path connecting the alpha and beta phases through an intermediate orthorhombic phase ($P2_12_12_1$), and find a surprisingly low barrier of $\sim$5 meV per formula unit. We note that a simple rigid-unit mode picture gives a good rough description of these energetics, and we map out the minimum-energy path in the space of rigid unit rotations in a physically insightful way.

Sinisa Coh
Department of Physics and Astronomy, Rutgers University

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