

Structural transitions in silica at Mbar pressures from ab initio metadynamics

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We present a study of structural transitions in silica at Mbar pressures by means of ab initio metadynamics technique. We find a series of structural transitions from the CaCl_2 -like phase to post-stishovite phases such as phases with kinked chains and the pyrite-like phase. This shows that the metadynamics algorithm is able to simulate also strongly reconstructive transitions in SiO_2 at extreme pressures. We analyze the observed transitions and describe their microscopic mechanisms.