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A first-principles investigation of ionic vacancies and diffusion in high-pressure silica polymorphs ASHOK VERMA, BIJAYA KARKI, Department of Computer Science, Louisiana State University, Baton Rouge, Louisiana 70803, USA — We have performed the density functional theory based simulations within the local density and pseudopotential approximations to investigate the effects of pressure and structural changes on the formation and migration energies of the ionic vacancies in crystalline silica. The simulations use supercells of 72 atoms for α-quartz, stishovite and $CaCl_2$-type and 96 atoms for α-PbO_2 and pyrite type silica. The simulations are performed up to 250 GPa pressure. The atomic positions are fully optimized. Our results show a discontinuous change in Schottky formation enthalpy at phase transitions which involve cation coordination number change. In fact increase in cation coordination number leads in reduction of Schottky formation enthalpy. For example, at 0 GPa pressure Schottky formation enthalpies of 4-fold (α-quartz), 6-fold (stishovite) and (6+2)-fold (pyrite) coordinated silica are 16.12 eV, 11.02 eV and 7.73 eV respectively. Calculations of migration enthalpies, activation enthalpies and activation volumes all are also carried out up to 250 GPa pressure.

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