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Vaporization of SiO_2 and $MgSiO_3$

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Vaporization is an important process in Earth's earliest evolution during which giant impacts are thought to have produced a transient silicate atmosphere. As experimental data are very limited, little is known of the near-critical vaporization of Earth's major oxide components: MgO and SiO_2. We have performed novel ab initio molecular dynamics simulations of vapor-liquid coexistence in the SiO_2 and $MgSiO_3$ systems. The simulations, based on density functional theory using the VASP code, begin with a suitably prepared liquid slab embedded in a vacuum. During the dynamical trajectory in the canonical ensemble, we see spontaneous vaporization, leading eventually to a steady-state chemical equilibrium between the two coexisting phases. We locate the liquid-vapor critical point at 6600 K and 0.40 g/cm^3 for $MgSiO_3$ and 5300 K and 0.43 g/cm3 for SiO_2. By carefully examining the trajectories, we determine the composition and speciation of the vapor. For $MgSiO_3$, We find that the vapor is significantly richer in Mg, O, and atomic (non-molecular) species than extrapolation of low-temperature experimental data has suggested. These results will have important implications for our understanding of the initial chemistry of the Earth and Moon and the initial thermal state of Earth.