Chemistry and Liquid-Vapor Phase Transition of $MgSiO_3$

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We report a benchmark study of liquid-vapor transition in a prototype silicate $MgSiO_3$ using the state of art first principles molecular dynamic simulations (FPMD) in terms of two-phase coexisting method (Heterogeneous). The liquid-vapor phase diagram of a silicate is established from heterogeneous FPMD methodology. The supercritical temperature of $MgSiO_3$ is found to be 6600 K with a critical density of 0.40 g/cm^3. Chemistry of vapor is characterized by studying the composition and speciation between 4000 K and 7000 K. We find O_2, SiO and SiO_2 are the most stable and abundant molecules in $MgSiO_3$ vapor. Our results clearly demonstrate the validity of methodology developed in current work and also provide the new opportunity to investigate the vaporization of other hot silicates (SiO_2 and hydrated $MgSiO_3$ liquids) in large impact events.