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# The critical point and the supercritical regime of MgO

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The position of the critical point determines the top of the liquid-vapor coexistence dome, and is a physical parameter of fundamental importance in the study of high-energy shocks, including those associated with large planetary impacts. For most major planetary materials, like oxides and silicates, the estimated position of the critical point is below 1 g/cm$^3$ at temperatures above 5000 K. Here we compute the position of the critical point of one of the most ubiquitous materials: MgO. For this, we perform first-principles molecular dynamics simulations. We find the critical density to be in the 0.4 - 0.6 g/cm$^3$ range and the critical temperature in the 6500 - 7000 K range. We investigate in detail the behavior of MgO in the subcritical and supercritical regimes and provide insight into the structure and chemical speciation. We see a change in Mg-O speciation towards lower degrees of coordination as the temperature is increased from 4000 K to 10000 K. This change in speciation is less pronounced at higher densities. We observe the liquid-gas separation in nucleating nano-bubbles at densities below the liquid spinodal. The majority of the chemical species forming the incipient gas-phase consist of isolated Mg and O atoms and some MgO and $O_2$ molecules. We find that the ionization state of the atoms in the liquid phase is close to the nominal charge, but it almost vanishes close to the liquid-gas boundary and in the gas phase, which is consequently largely atomic.

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