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The Critical Point and the vaporization of Phlogopite

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The Giant Impact event, in which a Mars-sized object collided with the proto-Earth, caused significant vaporization of the proto-Earth. The hot material generated from the Giant Impact formed a protolunar disk, which, upon cooling, condensed into the Earth and the Moon. Knowing the evolution of the liquid-vapor relations throughout this process is crucial for understanding the early evolution of the Earth-Moon system. So far, most of the studies addressed various oxides and silicate systems, all devoid of volatiles.

In this study, we investigate the critical point and vaporization of phlogopite as a model hydrous mineral. For this, we use molecular dynamics based on the density functional theory in the NVT ensemble (with fixed composition, volume, and temperature). We cover a wide range of densities (0.4 – 2.1 g/cm^3) and temperatures (2000 – 5000 K) relevant to the conditions of the protolunar disk. Our results show that the critical point of phlogopite can be well constrained to be between 4500 – 5000 K and 0.6 to 1.0 g/cm^3, as evidenced by the density-pressure plot at various temperatures. Furthermore, our simulations revealed the coexistence of melt and gas phases in the outer parts of the protolunar disk. We further analyze the composition and speciation of the liquid and gas phases at conditions relevant to the protolunar disk.

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