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Critical point of feldspars

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The main hypothesis for the Moon formation is the accretion of a debris disk formed after a Giant Impact between two large planetary embryos. For simulations modelling this impact and the subsequent accretion, one of the most important parameters is the position of the thermodynamic boundaries. Because of experimental difficulties few studies were done on the evaporation of silicates and none on feldspars even though they are the most abundant minerals in the Earth and Moon crusts.

Here we present our work on the three feldspar end-members, $KAlSi_3O_8$, $NaAlSi_3O_8$, and $CaAl_2Si_2O_8$. We perform *ab initio* molecular dynamics simulations in the canonical ensemble (constant temperature, volume and composition) using the Vienna Ab initio Simulation Package (VASP). We sample numerically a large range of temperatures and densities: from 3000 to 7000 K and from 1.1 to 6.4 g/cm^3. These ranges cover not only a large portion of the liquid state, but also the liquid side of the liquid-vapor dome and the position of the critical point, which we are searching for here.

We record the pressure and density for each simulation. We identify the minimum pressure at each isotherm, called liquid spinodal, which is the point at which the liquid becomes unstable. All the liquid spinodal points together give us the liquid spinodal line and the position of the critical point. We compare these results with those obtained for simpler materials. We monitor the fluid structure along with the atomic coordination and speciation, and compare the results obtained over the entire pressure and temperature ranges for the three end-members. Simulations at low densities display lasting voids with small clusters of atoms. This feature is thought to be a gas bubble nucleation and then indicates a two-phases region. The very first gas species formed during evaporation are identified and give new insight on the incongruent evaporation of silicates.

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