Supercritical silicate melts in the protolunar disk

Caracas Razvan*[1]

[1]CNRS, ENS de Lyon, Laboratoire de Geologie de Lyon (LGL) – CNRS : UMR5276 – CNRS, ENS Lyon, Laboratory of Geology of Lyon, France

Abstract

We employ large-scale molecular dynamics simulations to understand the physical and chemical behaviour of the magma ocean during the Giant Impact. We use the density-functional theory to compute the forces under which the atoms move according to Newtonian mechanics. For this we employ the VASP implementation.
Under pressure we find an increase of the coordination number of all atomic species, as a mechanism for accommodating compression, and a linear decrease of the self-diffusion. Iron atoms exhibit a gradual reduction of their magnetic moment.

We identify the supercritical region characterized by one homogeneous fluid, rich in ionic species. We show that the chemical speciation is very different from the one obtained at ambient pressure conditions. At lower temperatures, in the 2000 – 4000 K, we capture the nucleation of bubbles. When volatiles are present in the system, such molecular species, they are the first ones to evaporate and be present in these bubbles. We propose numerical tools to detect the liquid-vapor equilibrium. This is reached consistently regardless of the thermodynamic path.
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*Speaker