Geophysical Research Abstracts Vol. 20, EGU2018-13803, 2018 EGU General Assembly 2018 © Author(s) 2018. CC Attribution 4.0 license.



Ab initio molecular dynamics study of the supercritical state of Fe-based alloy

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The origin of the Moon is one of the oldest problem studied in Earth Sciences. The most widely accepted model today is that of a Giant Impact. According to this model an impactor hit the proto-Earth. The released energy was enough to melt and partially vaporize the two bodies; a large protolunar disk was generated from which the Earth–Moon couple formed.

Here we investigate the behavior of the core of the impactor during the impact, by computing the liquidvapour equilibrium and the supercritical point of Fe and Fe-based alloys. For this we employ first-principles molecular dynamics as implemented in the VASP package.

The simulations yield information on the equation of state of the melt and the supercritical fluid, and speciation of atoms in fluid phase. We also compute transport properties, like diffusion coefficients. Further we study the behavior or noble gases, like He in the molten Fe. We find it to be highly diffusive.