



First principles molecular dynamics study of the supercritical state of iron

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We investigate the behavior of the planetary iron-based cores of terrestrial bodies involved in Giant Impacts. We sample conditions similar to the ones that occurred prior to the formation of the protolunar disk. Due to poorly constrained equations of state and thermodynamic properties of iron in warm dense matter regime, the amount of vaporization of the two cores during impact is undetermined.

For this we employ first principles molecular dynamics simulations. We compute the equations of state of the liquid and of the supercritical fluids, we identify the position of the supercritical point, and we determine the entropy along the Hugoniot and the spinodal lines.

We find that our liquid-vapor equilibrium line is in a good agreement with available experimental data. We characterize the structural changes in the supercritical region by analyzing the speciation of atoms. Our results shed new light on the amount of iron vapor produced during the Giant Impact and provide new information on the equation of state and the thermodynamic properties of iron at high temperatures that may be used in future hydrodynamic simulations.

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