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Spin-polarized Molecular Dynamics simulations of liquid iron silicate at high pressures.

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Liquid iron silicate (Fe2SiO4) is an important component of natural silicate liquids appearing in Earth's interior. The effect of iron in the properties of these melts is a crucial issue, as it displays a high-spin to low-spin transition at high pressures which is accompanied by volume reduction and changes in the optical absorption spectrum. This phenomenon has a major influence on properties like the buoyancy or the thermal conductivity of the melt, and ultimately on the chemical and thermal evolution of our planet. Computer simulations using ab initio methods have proven to be a powerful approach to the study of liquid silicate systems[1,2], although not yet including Fe.

In this paper, we report ab initio molecular dynamics studies of liquid iron silicate at high pressure (up to 400 GPa) and high temperatures (from 3000K to 6000K) that allow us to predict different properties of the system. We use the spin-polarized formalism and the GGA+U density functional for a better treatment of the iron magnetic moments in the system. Previous studies in the solid phase have shown that GGA predicts fayalite as a metal, while the introduction of U leads to a correct description of the band gap and the magnetic ordering of the system. We extend this analysis to the liquid phase.

By means of these simulations we predict the liquid structure and thermodynamic properties of the liquid. We compute the theoretical Hugoniot for the system and find good agreement with values obtained from shock experiments [3]. Our calculations show large differences in the magnitude and orientation of the magnetic moments depending on the choice of functional; the GGA+U functional consistently provides larger values of the individual moments (about 1 unit larger) and of the total magnetization of the system. The high-spin to low-spin transition is predicted to take place at pressures from around 260GPa at 3000K to around 280GPa at 6000K in this iron-rich system.

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