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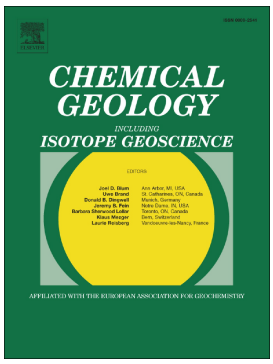

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Properties of planetary silicate melts by molecular dynamics simulation

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ABSTRACT

Because magmatic liquids play a fundamental role in the evolution of the terrestrial planets, a precise knowledge of their physical properties is requisite to better understand the formation and the dynamics of planetary interiors. In using an improved force field for silicates (Dufils et al., 2017), we report the results of a series of molecular dynamics simulations (MD) aiming to evaluate the equation of state (EOS), the viscosity, the electrical conductivity, and the elemental self-diffusion coefficients of various planetary melts representative of the Earth, Mars, the Moon and Mercury. The agreement between MD calculations and experimental data (when they exist) is remarkable, a finding which suggests that the MD simulations can be used on trust to extend the existing laboratory data on planetary melts (as it is proposed here for some lunar, martian and mercurian basalts) or to predict the thermo-physical properties of more exotic compositions (magma oceans, lava planets). Moreover, the MD simulations show that the evolution of the viscosity and of the electrical conductivity with the pressure depends in a complex manner on temperature and composition and that is difficult to extract general trends from these behaviors. Another advantage of the MD simulations is that the transport coefficients (viscosity, conductivity, and diffusivities) being evaluated along the same numerical experiment, one is able to test the validity of the Eyring and the Stokes-Einstein equations relating viscosity and diffusivity, as also as the Nernst-Einstein equation expressing the conductivity as function of the ionic diffusivities. It is shown that the Stokes-Einstein equation is suitable to describe planetary melts of low viscosity ($\leq$ 1 Pa.s), whereas the Eyring relation leads to a better estimation at high viscosities ($>$ 100 Pa.s). Concerning the electrical conductivity, the Nernst-Einstein relation fails to reproduce the conductivity values obtained by MD simulation, a result which can be explained by the crucial role played by ion-ion correlations in silicate melts.

***Keywords*:** Classical molecular dynamics simulations, planetary melts, EOS, viscosity, self-diffusion coefficients, electrical conductivity.