

Simulations of silicate and metallic melts for structural and dynamical insights

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Silicate magmas and metallic melts have played a crucial role in controlling the physical and chemical state of the Earth throughout its history. Understanding the behavior and properties of these melts at the pressure-temperature conditions that are relevant continues to be important but challenging research theme. To make significant progress in this endeavor, our approach has been computational, involving mostly first-principles molecular dynamics and now deep learning-based simulations, and also interactive visualization. Our analyses of simulation outputs for molten silicates, iron-rich alloys, and bulk Earth composition show that melt structure, density, and transport coefficients (including viscosity) vary considerably with both pressure and temperature. In this talk, we will touch upon some aspects of methodology, present selected results, and discuss their implications for partial melts in the mantle, early magma ocean dynamics, and core-mantle differentiation.