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Effects of temperature and pressure on the structure, transport properties and isotope fractionation in silicate melts GAURAV GOEL, JIM V. ORMAN, DANIEL J. LACKS, Case Western Reserve University — Knowledge of the physical and chemical properties of silicate melts is essential for understanding the properties and evolution of planetary interiors. In this talk we present results from extensive classical molecular dynamics simulations of silicate melts. These simulations were motivated by and provided insights into the laboratory experiments on magmatic systems. We have explored the effect of high temperature and high pressure, conditions typical of Earth's core-mantle boundary, on the relationship between transport properties and structure of silicate melts. We have also explored the role of melt structure and polymerization resulting from changing the melt composition, i.e. MgO/SiO₂ ratio. Finally, using non-equilibrium molecular dynamics simulations we investigated the effect of temperature gradient on isotopic fractionation in silicate melts.

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