Abstract Submitted
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First-Principles Molecular Dynamics of Melts in the MgO-SiO_2 System[1] BIJAYA KARKI, Louisiana State University, NICO DE KOKER, University of Michigan, D. BHATTARAI, Louisiana State University, LARS STIXRUDE[2], University of Michigan, DE KOKER COLLABORATION, STIXRUDE COLLABORATION — We have recently completed simulations of five melt compositions in the MgO-SiO_2 system within density functional theory. These results allow us to investigate the structural and thermodynamical, transport properties of melts along the MgO-SiO_2 join as a function of pressure. In particular, we have found that the mixing in MgO-SiO_2 system is significantly non-ideal at low pressures with negative excess volume and enthalpy of mixing. With increasing pressure, the volume of mixing decreases rapidly to a value close to zero at pressures above 50 GPa whereas the enthalpy of mixing remains negative. The radial distribution functions and coordination environments are found to show interesting changes with varying composition. Also, the effects of composition on diffusivity are shown to be substantial at low pressures whereas the effects are increasingly suppressed with increasing pressure.

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