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Silicate melts of the Earth's mantle

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We explore the state of various silicate melts, with different realistic compositions, characteristic for various moments of the crystallization of the magma ocean. Using a starting basis of silica tetrahedra we vary the amount and the quality of the cations, including trace elements.

For this, we employ first-principles molecular dynamics simulations. We perform spin-polarized calculations in the planar augmented wavefunction formalism of the density-functional theory, using the VASP package.

We monitor the dependence with pressure and temperature of various physical parameters, like density, coordination number, magnetic spin, viscosity, etc. We show that the coordination number in the silicate groups increases from 4 to 5 to 6 as we go from ambient pressure to megabar. We estimate the thermal dilatation; from the equations of state we compute the velocities of the compressional seismic waves. We use these results to show that melts can still exist at the base of the Earth's present-day lower mantle as iron-rich pockets. These melts can explain particular features, characterized by low seismic velocities, such as the ultra-low velocity zones. Using the more complex chemistries we provide the first insights into the behavior of the magma ocean during cooling and crystallization.

Keywords: mantle, silicate, melt, spin transition, equation of state, magma ocean