Minor elements in silicate melts from ab initio calculations

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We study the behavior of trace elements, *i.e.* Ni, Co, W, etc. in silicate melts and their partitioning with metallic melts using first principles molecular dynamics calculations. We use the V.A.S.P. the package with the planar augmented wavefunction (PAW) formalism of the density functional theory.

A clinoenstatite supercell containing 160 atoms was created and subsequently melted by heating using a Nose-Hoover thermostat at 5000 Kelvin and around 25 GPa. After melting, the melt was cooled to 3000K and trace amounts of Ni were added. We vary the composition of major cations in the melt by exchanging Mg with Fe. Here Fe enters as ferrous iron. We study the melt compression along the 3000K up to 150 GPa. We look at the effect of the Fe^{2+} spin transition on the melt polymerization, the formation of coordination polyhedra, the diffusion coefficients, and the Ni solubility.