# First-principles computation of mantle materials in crystalline and amorphous phases

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Over the last two decades, first-principles methods based on density functional theory have widely been used to study the behavior and properties of mantle materials over broad ranges of pressure, temperature, and composition that are geologically relevant. The calculated properties include structure, phase transition, equation of state, thermodynamics, elasticity, alloying, conductivity, defects, interfaces, diffusivity, viscosity, and melting. Considering MgO and major silicate materials, we have found that most properties are strongly pressure dependent, sometimes varying non-monotonically and anomalously, with the effects of temperature being systematically suppressed with compression. The overall agreement with the available experimental data is excellent. Here, we review the results from first-principles molecular dynamics simulations of silicate liquids in $MgO$-$CaO$-$FeO$-$Al_2O_3$-$SiO_2$-$H_2O$ system with focus on structure, density, and transport properties. These melt properties have been important to our understanding of the origin, stability and mobility of melts in the modern Earth as well as early magma ocean dynamics and cooling.