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First Principles Molecular Dynamics Simulations of Diopside Liquid at High Pressure NI SUN, LARS STIXRUDE, University of Michigan, BIJAYA KARKI, Louisiana State University — Diopside ($CaMgSi_2O_6$) is a major component of basalt; the high-pressure end members, Mg-perovskite ($MgSiO_3$) and Ca-perovskite ($CaSiO_3$), make up more than 80 % of the lower mantle. Despite its importance, most studies of diopside liquid have been performed at relatively low pressures and temperatures. In this study, we investigated $CaMgSi_2O_6$ liquid at lower mantle conditions by first principles molecular dynamics (FPMD) simulations based on density functional theory. The average Si-O coordination number increases nearly linearly from 4 to 6 with two-fold compression. The structure shows evidence of incipient exsolution with non-random clustering of Mg and Ca ions. Our results are well fitted by Mie-Grüneisen equation of state with a Grüneisen parameter that increases on compression. The variation of the diffusion coefficient with pressure and temperature is captured by the Arrhenius relation with activation energy and volume $E^* = 1.2$ eV and $V^* = 1.25$ Å^3. The electronic properties of the $CaMgSi_2O_6$ liquid phase are similar as those of the $MgSiO_3$ liquid: there is no band gap and an extra peak appears at the Fermi level at low pressure.

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