

## First principles simulations of model basalt melts at high pressure

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Towards sampling compositions comparable to natural magmas, we have recently simulated model basalt melt system, which consists of four most common components (MgO, CaO, Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub>) with/out H<sub>2</sub>O. Our first principles simulations suggest that the melt structure is controlled by cation-anion bonding to show strong short-range order. As pressure rises, the structure changes considerably with all cation-anion coordination numbers increasing relatively rapidly initially and then gradually at pressures above 50 GPa. The predicted trend is consistent with experimentally inferred pressure behavior of Si-O coordination of basalt melt. When compared with other silicate liquids, we notice an interesting trend that the effects of composition on the mean cation-anion coordination are rather small implying that the corresponding coordination polyhedra serve as building blocks of silicate melts. How these structural units exist and how they act together to control the melt behavior perhaps vary among different melts. For instance, these units are interlinked to varying degree in different liquids. The simulated model basalt melts contain less than 70 % bridging oxygens even when both Si and Al are together considered as network formers. Simulations of hydrous basalt melt show that water dissolves in the form of hydroxyls and water molecules at low pressure and as more extended structures at high pressure. The system commences to behave ideally at pressures above 10 GPa, a similar behavior with much higher pressure of 50 or above was predicted for hydrous SiO<sub>2</sub> and MgSiO<sub>3</sub> melts. This implies an unlimited solubility of water in silicate melts, and the water solubility rather appears to be insensitive of composition at high pressure. Also, proton diffusivities for different melts agree mostly except at low pressure-low temperature regime where hydrous silica liquid show much slower diffusion.