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**Water in MgSiO<sub>3</sub> melt at high pressure** MAINAK MOOKHERJEE, LARS STIXRUDE, University of Michigan — The presence of water is thought to play important role in modifying the equilibrium and transport properties of earth materials including silicate liquids. In our study we want to address the following questions: How does the presence of water modifies density of melts? What is the partial molar volume of water in melts? What structural species of H<sub>2</sub>O are present at high pressure? In order to address these issues we explore the high-pressure behaviour of hydrous MgSiO<sub>3</sub> melt with 11 wt% H<sub>2</sub>O, using first principles molecular dynamics simulation, based on local density approximation (LDA) and the plane-wave-pseudopotential method. The simulations are performed in the canonical ensembles with periodic boundary conditions and a Nose' thermostat. Melting was confirmed by the radial distribution function displaying no long-range order. By comparing our results with that of the anhydrous counterpart (Stixrude and Karki, 2005), we find that the partial molar volume of water decreases along the 3000 K isotherm from 20 cc/mol at 2 GPa to 6.6 cc/mol at 80 GPa. The water component is substantially more compressible than the silicate component. The partial molar volume of water is much less than the volume of pure water at the same conditions (Pitzer and Sterner, 1994), indicating a difference in structure. Analysis of our simulations shows a range of H<sub>2</sub>O species including hydroxyls, water molecules and H-O-H-O groups.

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