

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Structure and freezing of MgSiO<sub>3</sub> liquid in Earth's interior** BI-JAYA KARKI, Louisiana State University, LARS STIXRUDE, University of Michigan — Silicate liquids are primary agents of mass and heat transport, yet little is known of their physical properties or structure over most of the mantle pressure regime. We have applied density functional theory within the local density approximation to the study of silicate liquids via Born-Oppenheimer first principles molecular dynamics. The simulations are performed in the NVT ensemble with a Nose thermostat. We find that over the pressure regime of Earth's mantle the mean Si-O coordination number increases nearly linearly with compression from four-fold to six-fold. The Grüneisen parameter of the liquid increases markedly on compression, in contrast to the behavior of mantle crystalline phases, and in accord with expectations based on the pressure-induced change in structure of the liquid. The density contrast between liquid and crystal decreases nearly five-fold over the mantle pressure regime and is 4 % at the core-mantle boundary. The melting curve, obtained via integration of the Clausius-Clapeyron equation yields a melting temperature of  $5400 \pm 600$  K at the core mantle boundary. Our results support the notion of buoyantly stable silicate melts at the core-mantle boundary.

Lars Stixrude  
University of Michigan

Date submitted: 27 Nov 2005

Electronic form version 1.4