Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Thermodynamics of Mg_2SiO_4 liquid from first principles molecular dynamics simulations NICO DE KOKER, LARS STIXRUDE, University of Michigan — As the main medium through which planetary differentiation occurs, silicate liquids have a central role in the study of the Earth. We determine the structural and thermodynamic properties of Mg_2SiO_4 liquid using first principles molecular dynamics in the framework of density functional theory and the local density approximation (LDA). Calculations, performed in the canonical ensemble with a Nose thermostat, span a range of pressures (0 - 150 GPa) and temperatures (3000 - 6000 K). Simulations are performed over 3000 time steps (femto seconds), yielding the total energy and average pressure from which the equation of state, heat capacity and Gruneisen parameter are determined. Preliminary results show that, in addition to the increase in Si coordination with pressure, about one third of the O atoms are not bound to Si at low pressure, a fraction which vanishes with increased Si coordination.

Nico De Koker
University of Michigan

Date submitted: 28 Nov 2005 Electronic form version 1.4