Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Thermoelasticity of Al^{3+}- and Fe^{3+}-bearing bridgemanite[1] JUAN VALENCIA-CARDONA, GAURAV SHUKLA, University of Minnesota Twin cities, MATTEO COCOCCIONI, Ecole Polytechnique Federale de Lausanne, Switzerland, RENATA WENTZCOVITCH, University of Minnesota Twin cities — We present quasi-harmonic LDA+U calculations of thermoelastic properties of Fe^{3+}- and Al^{3+}-bearing bridgemanite ($MgSiO_3$), the main Earth forming phase, at relevant P,T conditions and compositions. Three charge-coupled substitutions, namely, Al^{3+}-Al^{3+}, Fe^{3+}-Fe^{3+}, and Fe^{3+}-Al^{3+} have been investigated. Aggregate elastic moduli and sound velocities are successfully compared with limited experimental measurements available. The effect of the pressure induced high-spin to low-spin state change in Fe^{3+} in the B-site has been investigated in great detail since it has potentially dramatic effects on seismic velocities in the Earth's lower mantle.

[1]Research supported by NSF/EAR and NSF/CAREER

Gaurav Shukla
University of Minnesota Twin cities

Date submitted: 14 Nov 2014 Electronic form version 1.4