

Effect of spin transition on the elasticity of magnesiumwustite

Taku Tsuchiya[1]; Cesar da Silva[2]; Renata Wentzcovitch[3]

[1] GRC, Ehime Univ; [2] MSI, U of Minnesota; [3] CEMS, U of Minnesota

Iron in the major lower mantle (LM) minerals undergoes a high spin (HS) to low spin (LS) transition at relevant pressures (23-135 GPa). Using the LDA+U with internally consistent U, we have successfully reproduced this transition in low solute concentration magnesiowustite, $(\text{Mg}_{1-x}\text{Fe}_x)\text{O}$, (x less than 0.2), the second most abundant LM phase. The HS-LS transition goes through an insulating (semiconducting) intermediate mixed spins (MS) state without discontinuous changes in properties at high temperatures. We also found that this transition is accompanied with large volume reduction and thus considerable change in elastic property. These encouraging results indicate that our method enables first principles studies of strongly correlated iron-bearing minerals, a major class of mineral physics problems.

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