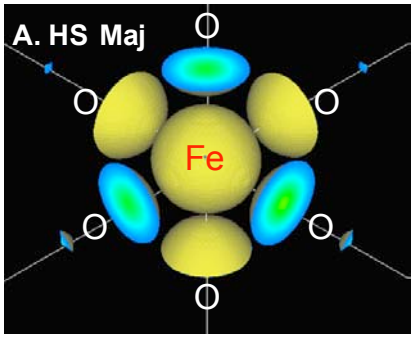
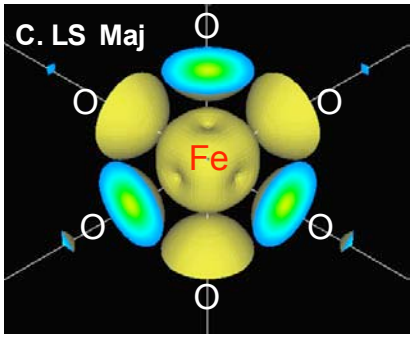
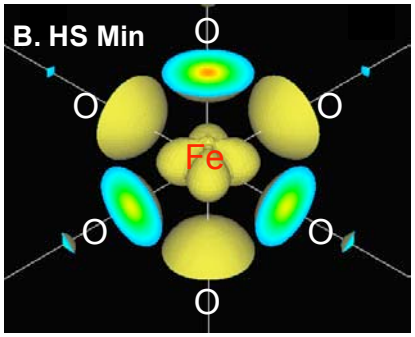
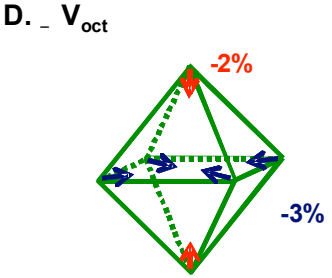
Institute for the Theory of Advanced Materials in Information Technology: James R. Chelikowsky (Texas), Yousef Saad and Renata Wentzcovitch (Minnesota), Steven Louie (UC Berkeley) and Efthimios Kaxiras (Harvard) (DMR- 0551195): Spin transition in complex oxides under pressure

Fe-Mg oxides may undergo a high spin (HS) to low spin (LS) transition under pressure (23-135 GPa). Previous first principles methods have failed to describe this phenomenon. Using a new rotationally invariant formulation of density functional theory (LDA+*U)*, we were able to describe successfully this transition in the low solute concentration for the oxide: magnesiowüstite (Mw), $(Mg_{1-x}Fe_x)O$, ($x < 0.2$). We show that the HS/LS transition goes through an insulating (semiconducting) intermediate mixed spins state without discontinuous changes in properties, as seen experimentally. These encouraging results open for exploration by first principles a new class of spin related phenomena.









Charge densities around a ferrous iron in magnesiowüstite. Isosurface charge densities with $\rho = 0.3$ e/Å^3 for majority (A) and minority HS (B), and majority/minority LS (C). Polyhedral volume collapse across the spin transition (D). Six caps surrounding the ferrous ion belong to oxygens.