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FeO under Zero and High Pressure Conditions – coupling first principles with numerical models

M. Alfredsson, S. Stackhouse, G.D. Price and J.P. Brodholt

Dept. of Earth Sciences, University College London, Gower Street, London, WC1E 6BT, UK (m.alfredsson@ucl.ac.uk)

Determining the effect of Fe on the chemical and physical properties of lower mantle minerals is fundamental to interpreting lower mantle seismic data. While ab initio computaional modelling has proven to be an invaluable tool for Fe-free systems, there are serious problems with these techniques when applied to transition metal oxides (ref to Cohen). For example, Density Functional Calculations (DFT) predict FeO to be metallic when in fact it is a wide band-gap insulator.

In this study we use different hybrid functionals between Hartree-Fock and DFT as an alternative to the traditional approaches of LDA+U and Self-configuration interactions (SIC) calculations. We determine the geometrical and electronic structures and bulk properties of different magnetic and crystallographic structures of FeO, and find that the different functionals predict quite different elastic properties. By comparing with available electronic and structural experimental data, we propose an optimum range of mixing between HF and DFT.

Using the hybrid functionals it is demonstrated that FeO undergoes two pressure-induced phase transitions in the range of 0-150 Gpa. Firstly at 85 GPa the rhombohedrally distorted anti-ferromagnetic B1 (r-B1)(AFM)) structure undergoes a structural phase transition into an inverse-B8 structure. Increasing the pressure further, i-B8(AFM) structure polymorph transform into a non-magnetic B8 structure. Hence, the latter phase transition is coupled with a magnetic transition, i.e. the Fe-ions change their spin state from a high-spin to low-spin configuration. Experimentally the reported observations disagree with each other - M?ssbauer measurements report a high spin to low spin transtion between 90-140 GPa (Pasternak MP et al. (1997) PR Letters. 79: 5047-5049), while X-ray emission spectroscopy suggest a preserved high spin

state up to 143 GPa (Badro J et al. (1999) PR. Lett. 83: 4101-4104).

After determine the existing polymorphs as a function of pressure, we have calculated the elastic constants for them. In agreement with the experimental study by Jacobsen and co-workers (S.D. Jacobsen et al. (2004) PNAS, 101:5867-5871) we find that C_{44} in the B1-structure is elastically instable, reported as a mode softening of C_{44} as a function of pressure.

Finally we will discuss how the structural and elastic properties determined from our first principles calculations on FeO can be coupled with numerical models (via the Christoffel equations) to predict the compressional and shear wave velocities of the deep Earth.