DFT+U equation of state for iron oxide

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The number of detected exoplanets and the capabilities of identifying small, Earth-sized planets have grown tremendously over the last two decades. Yet many of those Earth-sized planets are only characterized in mass and radius. Therefore, interior structure models rely heavily on equations of states (EOS) for rock material to characterize the planetary properties. One particular interesting material is iron oxide, which is very challenging to treat with standard Density Functional Theory (DFT) methods. Here we investigate the DFT+U approach to obtain the correct electronic and structural properties for the FeO phases typically predicted at the high pressures within the planetary interiors. The Hubbard U is obtained self-consistently from spin-polarized DFT calculations with QUANTUM ESPRESSO [1,2] using the linear response approach [3]. The resulting optimized ground state is used as a starting point for phonon calculations within the quasi-harmonic approximation. Based on these calculations we investigate the impact of the Hubbard U on the EOS providing a step forward to incorporating more realistic rock material into interior structure models of super-Earths.

REFERENCES

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