

LDA+U calculation of Iron-containing Minerals

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The evolution of magnetic properties of minerals with pressure and their interplay with structural and elastic properties is a fascinating geophysical and material science subject. As many mineral phases, containing transition metal elements, are Mott insulating and ordinary band structure methods fail to properly account for their electronic behavior there is a need to integrate the DFT band structure description with more correlated approaches.

In the last ten years LDA+U [1-2] has been proposed as an alternative to more traditional LDA/GGA approximations for strongly correlated systems. Yet its application to the study of structural properties of materials has been only sporadic, in part due to the technical difficulty in computing atomic forces within the all-electron methods usually employed in the calculation. Moreover, more often than desirable, the parameters defining the functional have not been obtained from first-principles.

We have implemented the LDA+U method in a state-of-the-art plane-wave pseudopotential code (PWscf, distributed under the Gnu GPL licence at the site <http://www.pwscf.org>). Moreover, a consistent way to determine the Hubbard U parameter entering the functional have been devised, extending the original approach [3], valid only in a LMTO framework, to a plane-wave pseudopotential formalism.

The structural and magnetic properties of a prototype system, low pressure FeO, have been addressed, clarifying the importance of orbital ordering for the stabilization of the correct magnetic ground state of the system and for the pressure evolution of its structural properties. The method has then been applied to Fe₂SiO₄, Fayalite, the Iron-rich end member of the Iron-Magnesium olivines present in the Earth upper mantle. Also in this case the electronic properties are dramatically improved with respect to the LDA/GGA results.

This work has been done in collaboration with Matteo Cococcioni at SISSA and DEMOCRITOS, Trieste, Italy.

[1] V.I. Anisimov, J. Zaanen, O.K. Andersen, Phys. Rev. B **44**, 943 (1991).

[2] A.I. Liechtenstein, V.I. Anisimov, J. Zaanen, Phys. Rev. B **52**, R5467 (1995).

[3] V.I. Anisimov, O. Gunnarson, Phys. Rev. B **43**, 7570 (1991).

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