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Electronic structure and phase transition in iron bearing minerals

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First-principles calculations are playing an important role in the development of our understanding of Earth interior. A proper treatment of iron bearing minerals is fundamental in this respect. Unfortunately standard DFT approaches such as the local density (LDA) or generalized gradient (GGA) approximations fail in describing even qualitative features of even simple iron minerals, such as the insulating nature and magnetic structure of many oxides. DFT+U approximation has demonstrated to improve significantly the physical description of transition metal and rare earth compounds. In order to make DFT+U a really "ab-initio" approach, an internally consistent determination of the involved U parameter is however needed. In alternative computationally more demanding, but supposedly more accurate, approaches such as PBE0 or B3LYP Hartree-Fock-DFT hybrid functionals can be explored. I'll report on my recent research on these subjects, focussing on iron oxide, magnisium-wustite high-spin-low-spin phase transition, and ematite.