Abstract Submitted
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New perspectives in transition metal compounds' design from first-principles calculations[1] MATTEO COCOCCIONI, DMSE and ISN, Massachusetts Institute of Technology — Transition-metal (TM) compounds are involved in many important physical processes and chemical reactions (such as minerals in the earth's mantle, Li ion batteries' cathodes, spintronics, catalysis on surfaces, chemical reactions on biomolecules). Unfortunately, standard DFT approaches are often not quantitatively accurate for these materials, due to the poor representation of electronic correlation. We address several of these problems by establishing a parameter-free approach to the GGA+U method. The Hubbard U is defined and obtained through a fully self-consistent linear-response approach. An accurate description of TM compounds under different conditions is obtained; examples are given for a) ground state and structure of FeO under pressure, b) voltages, stability and conduction properties of cathode materials such as olivine, layered and spinel TM compounds, and c) valence state and coordination for solvated aqua iron ions.

[1]Work done in collaboration with:
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