Electronic Structure Of Transition Metal Elements In Oxides And Semiconductors: The Self-Interaction Corrected Local Spin Density Methods

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The local spin density approximation to density functional theory has proven an extremely powerful method to study the ground state electronic and magnetic structure of transition metals. It has, however, been less successful in describing transition metal (impurities) in oxides and semiconductors, where it often predicts incorrect magnetic ground states. This failure is often attributed to the in proper treatment of electron correlations in systems with localized orbitals and is commonly corrected with an empirical local Coulomb repulsion term (LDA+U methods). We will discuss a different approach to this problem. It is based on the recognition that approximations to the exchange and correlation potential introduce spurious self-interaction that overestimate the hybridization of localized orbitals with the host electrons. A self-interaction free functional that is still based on the local density approximation was proposed some twenty years ago by Perdue and Zunger [PRB 23, 5048 (1981)] and has been shown to have all the "nice" properties of LSDA. Practical schemes to minimize this functional in solids emerged about a decade later [Svane and Gunnarsson, Phys. Rev. B 37, R9919 (1988); Temmerman et. al., Phys. Rev. B 47, 1184 (1994)] and have been used successfully in actinides and transition metal oxides.

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