

Electronic Structure of Dilute Magnetic Semiconductors: A Comparison of the SIC-LSD and the LDA+U Methods

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The Local Density Approximations (LDA) to Density Functional Theory is one of the most successful approaches to compute materials properties from first principles. However, when applied to systems with localized orbitals, such as antiferromagnetic insulators or dilute magnetic semiconductors, the method fails to predict basic ground state properties. Two fairly efficient extensions that are tailored for solids with strongly correlated electrons has been developed over the last two-decade. The first is the LDA+U method, in which an ad hoc on-site Coulomb repulsion for localized orbitals is added to the density functional. This method, which is inspired by the Hubbard model, successfully describes the magnetic and spectroscopic properties of transition metal oxides. The second method is the Self Interaction Corrected (SIC) Local Spin Density (LSD) method, in which the spurious self-interactions of the LDA are subtracted from the density functional. The SIC-LSD is parameter free, successfully describes ground state properties of oxides, but has been criticized for failing to predict the position of localized levels in photoemission spectra.

We apply the SIC-LSD method to study the electronic structure and magnetic properties of Mn-doped III-V semiconductors, a new class of materials with intriguing magnetic properties. We compare the results with previous LDA and LDA+U calculations that have so far failed to properly describe the Mn-d orbitals. A proper description of these orbitals is key to understanding of magnetic exchange in these materials. We find, that the SIC-LSD method correctly predicts the p-d exchange strength, and hence Curie temperatures of Mn doped GaAs. We were also able to perform fully self-consistent Δ -SCF calculation and predict the position of the photoemission peak of the localized levels.

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