Transition metal ions in semiconductors: LDA, LDA+U, and experiment

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The known failure of the Local Density Approximation (LDA) is the underestimation of the band gap in solids, ascribed to the oversimplified treatment of exchange-correlation effects, and particularly drastic in transition metal (TM) oxides. A considerable improvement is obtained by adding the +U correction for particular atomic orbitals. While the impact of +U terms was extensively discussed for ideal crystals, its impact on the electronic structure of defects is less understood. We analysed the impact of the +U term for Cr, Mn, Fe, and Co ions in GaN and AlN. The +U term was treated as a free parameter, and it was applied to p(N) and d(TM) orbitals. The results of LDA+U calculations were compared to available experimental data. The band gap of GaN is correct with U(N)=4 eV. The +U terms strongly affect the electronic structure of TM impurities. Surprisingly, for U(TM)=0, the energies of the gap levels induced by these centers, and of the intra-center optical transitions, agree well with experiment. In contrast, for U(N)=U(TM)=4 eV, these energies are in substantial disagreement with experimental values by about 1-2 eV.

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