Electronic structure calculations of transition metal and rare earth nitrides using LSDA+U

Aditi Herwadkar, Paul Larson and Walter R.L. Lambrecht

Department of Physics, Case Western Reserve University
Cleveland, OH, USA

Electronic structure calculations within the local spin density approximation (LSDA) have limitations dealing with highly localized orbitals, such as d and f states. LSDA+U calculations allow to add a Hubbard U correction self-consistently to obtain the correct position of these localized states. A series of calculations have been performed with LSDA+U on rocksalt nitrides using the linearized muffin tin orbital (LMTO) method. CrN has an observed optical gap of 0.7 eV though LSDA predicts a metal. Addition of LSDA+U in the fully localized limit opens a gap while changing the order of the states near the Fermi level which makes it a charge transfer type Mott-insulator. Similar calculations were performed on the rare-earth (Ce-Lu) nitrides. The f orbitals are highly localized and become pinned at the Fermi level. Addition of LSDA+U moves the states away from the Fermi level. Within the rocksalt symmetry, the f orbitals split into two triply degenerate t_{1u} and t_{2u} states and a nondegenerate state a_{2u}. The f orbitals prefer to remain completely empty or completely filled. In cases with 2 or 5 extra electrons, such as PrN, SmN, DyN, and TmN, partial filling is only possible, leading to heavy-Fermion behavior. This work is supported by ONR and NSF.