Abstract for an Invited Paper
for the MAR10 Meeting of
The American Physical Society

Applications of LSDA+U to defects in semiconductors and calculation of magnetic exchange interactions

WALTER LAMBRECHT, Case Western Reserve University

The LSDA+U (local spin density approximation with Hubbard-U corrections) was originally introduced for systems with narrow bands and strong Coulomb interactions. However, it can also be used in a somewhat empirical manner to generate an orbital dependent shift potential to correct LDA band gap underestimates. In this talk I will discuss some aspects of LSDA+U. For example, does LSDA+U give a unique solution? How to choose U? What are the various flavors of LSDA+U? I will show that the ground state of rare-earth nitrides in LSDA+U depends on the symmetry of the starting density matrix and how this relates to Hund's rules and orbital magnetic moment. I will then show how we can use this approach to calculate exchange interactions in Gd pnictide compounds. In combination with the Liechtenstein linear response approach, we calculated exchange interactions in Mn-doped ScN and in Gd pnictides. In those examples we used not only the Uf for f electrons but also a Ud to shift the d-like conduction band up. In a similar manner, we used a Us to shift up the bottom of the s-like conduction band in ZnO and used this approach in an attempt to clear up the controversies over the oxygen vacancy level in ZnO. I will discuss the relation of this approach to other band gap correction approaches such as hybrid functionals and GW. It appears important to not only correct the minimum gap but the gap at various k-points and in fact separately the two band edges. Work along those lines is in progress.