Vacancies and Impurities in Semiconductors

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On the example of oxygen vacancies (F-centers) [1] and transition metal impurities [2] (diluted magnetic semiconductors (DMS)) in ZnO we show the capability of ab initio embedded cluster calculations for the treatment of semiconductors. We applied wavefunction based multireference methods (CASSCF) on the ab initio cluster. This guaranties a correct description of the spin states in the ground state as well as the excited states.

For the magnetic exchange coupling between two transition metal centers it was necessary to include orbital relaxation effects in charge transfer configurations, i. e. configurations in which one TM center is in oxidation state I and another in oxidation state III. This was taken into account by a modified valence CI.

Furthermore, we investigated the influence of spin orbit coupling (SOC) on the electronic states. SOC is usually not included in plane wave DFT band structure calculations which are the standard theoretical approach on DMS. In case of Ni doted ZnO it proved necessary to include SOC for receiving the correct ground state.

To obtain accurate transition energies of F centers we had to consider geometric relaxation of the first Zn shell. Dynamic correlation of the vacancy electrons as well as the first Zn shell (4 atoms) and the first O shell (12 atoms) was included by incremental MCCEPA calculations.

References

[1] Fink, K. *Phys. Chem. Chem. Phys.* **2005**, *7*, 2999-3004.
[2] Fink, K. *Chem. Phys.* **2006,** in press.