**Chemical Bonding Based on Charge Density Calculations for Solids**

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We calculate the electronic structure of solids within density functional theory (DFT) and use the WIEN2k code [1] that is based on the full-potential augmented plane wave (APW) method. The key quantity is the electron density, which can be decomposed into contributions according to core and valence regions or even a small energy region (an energy sub band) that gives more insight into the chemical bonding than the total density. The partial densities of states (DOS) partitioned into atomic ℓ- and m-like contributions provide further details in chemical bonding.

Recently the experimental determination of the electronic charge density has been greatly improved, e.g. due to synchrotron radiation which allows to obtain structure factors with high accuracy [2]. Although the comparison between theory and experiment is made difficult by T=0 calculations vs. finite temperature experiments with absorption and extinction, fine details can be extracted that often agree well and lead to a better understanding of chemical bonding.

Such comparisons will be shown for a selected class of materials from oxides, $SiO_2$, silicates to highly correlated systems as the high-temperature superconductor $YBa_2Cu_3O_7$ [2] or the pyrochlore compound $Y_2Nb_2O_7$ [3]. A special feature appears in $BaCoO_3$ for which orbital is found to occur along the Co chains.

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