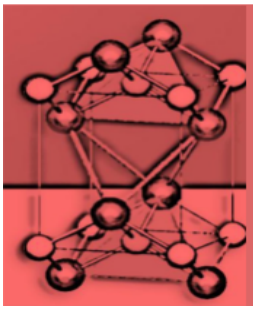

IX Workshop on Novel Methods for Electronic Structure Calculations

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DFT as a tool for electronic structure calculations for solids

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Density functional theory has become the de facto standard for electronic structure simulations in materials science. However, the accuracy and predictability of DFT calculations still depend on the approximate functional in use and unfortunately different material classes and even different properties like formation energies or band gaps may require different approximations. It is thus very advantageous to know for which material class certain DFT functionals perform well and what accuracy/errors one can expect. Even using the most advanced meta-GGAs like the famous SCAN functional, particular challenging are systems with transition metal atoms because of possible strong d-d correlations or van der Waals systems with very weak, but still essential interactions. For testing new functionals an accurate all-electron method like the APW-lo method as embodied in the WIEN2k code provides unbiased results. I'll also demonstrate that the power of DFT nowadays also extends to finite temperature properties and discuss temperature induced phase transitions in $BaTiO_3$ or the effect of phononson the B-K edge spectrum ofhexagnal BN.