MAR11-2010-002496

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

The shortcomings and advantages of hybrid functionals in the description of solids[1]

GEORG KRESSE, University of Vienna

For extended systems, density functional theory currently possesses the optimal balance between computational efficiency and accuracy. Hence its wide spread acceptance and application in quantum chemistry, materials science and computational catalysis is in no way astonishing. However, it is also well known that standard density functionals underestimate the band gap in particular for small gap systems, and resultantly structural properties related to the band gap are difficult to predict. In quantum chemistry this has long be realized, and hybrid functionals mixing Hartree-Fock and local density functionals are generally preferred over purely local functionals. Such functionals usually predict a much larger band gap than purely local density functionals. With the exception of the Crystal code, hybrid functionals were not available in popular periodic codes, and only recently successful implementations and applications using plane wave based codes, such as VASP, were reported. In this talk, I will survey the expertise we have acquired for hybrid functionals for extended systems. For simple prototypical materials, such as metals, semiconductors, and insulators many ground state properties are indeed found to be in much better agreement with experiment than using purely local functionals. This concerns lattice constants and bulk moduli, but phonon dispersion relations are also often significantly improved, in particular, for those semiconductors where DFT predicts no band gap. Some specific applications will be discussed in detail. This includes the description of (small) polarons in semiconductors, the properties of ferroelectric materials (specifically $BaTiO_3$ and $SrTiO_3$), phonon dispersion relations in the group IV elements, and magnetic impurities in semiconductors.

[1]Support by the Austrian FWF is acknowledged