SUMMER SCHOOL: BANDSTRUCTURE MEETS MANY BODY THEORY

18. SEPTEMBER 2012 – 22. SEPTEMBER 2012 IN VIENNA, AUSTRIA

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A particular challenge of computational materials science is the calculation of materials in the presence of strong electronic correlations and exchange. In this case, the local density approximation (LDA) or generalized gradient approximation to the exchange correlation potential often yields unreliable results. In recent years we have seen tremendous progress in this field: Hedin's GW approximation which, at its core, replaces the exact exchange by a screened exchange, matured to the point that calculations are routinely feasible, and in most program packages the required routines are now available. Screened exchange contributions are also included in computationally less demanding hybrid functionals, giving often reliable structural predictions. Unfortunately strong correlation, correlated metals as well as the description of the paramagnetic insulating state are usually not captured by these approaches. Density matrix renormalization group and related matrix product states, novel quantum Monte Carlo algorithms, and dynamical mean field theory are needed to complement the other methods.
Scientists from the bandstructure and from the many body community have joined forces, combining the most successful approaches of the two respective communities, as for instance exemplified by the LDA+DMFT approach. The aim of the Summer School is to educate the next generation of scientists in both, bandstructure and many body theory. To this end, we will have lectures in the morning and hands-on tutorials in the afternoon on the following topics:

- local density approximation (LDA)
- exact exchange
- quantum chemistry approaches (CI and active space techniques)
- GW
- dynamical matrix renormalization theory (DMRG)
- Quantum Monte Carlo (QMC)
- Dynamical mean field theory (DMFT)
- combining methods: LDA+DMFT and GW+DMFT

Invited speakers (prospectively):

◆ C. Ambrosch-Draxl (Berlin) LDA ◆ S. Biermann or A. Georges (Paris) GW+DMFT
◆ P. Blaha (Vienna) LDA, LDA+U ◆ R. Godby (York) or L. Reining (CNRS Paris) GW
◆ E.K.U. Gross (MPI Halle) or K. Burke (UC Irvine) TDDFT
◆ M. P. Head-Gordon (Berkeley) or F. Manby (Bristol) quantum chemistry
◆ J. Kunes (Prague) Wannier functions ◆ M. Towler (Cambridge) QMC
◆ U. Scalettar (Davis) lattice QMC ◆ D. Vollhardt (Augsburg) DMFT