Ab initio Studies of Excited-State Phenomena in Condensed Matter: GW, GW-BSE, and Beyond

A talk by Steven G. Louie

Univ of California at Berkeley & Lawrence Berkeley National Laboratory, USA

DATE / TIME: Tuesday, April 4th 2017, 4:45 p.m.

LOCATION: Christian-Doppler-Hörsaal, Boltzmanngasse 5, 3. Stk., 1090 Wien

Many fundamental phenomena in and applications of materials are dictated by the nature of their excited states. In this talk, we discuss some recent progress and applications of the GW approach and its extensions to compute electronic excited-state properties, in particular of reduced-dimensional systems. This approach of many-body perturbation theory incorporates electron-electron interaction through the screened Coulomb interaction W, considering successively higher-number interacting particle Green's functions. Quasiparticle excitations are computed within the GW approximation, and 2-particle excitations (e.g., those in optical responses) within the GW plus Bethe-Salpeter equation (GW-BSE) method. Many-electron effects are particularly important in reduced-dimensional systems, where together with symmetry, dimensionality and screening effects can lead to important new concepts and novel phenomena. We illustrate this with several examples of current interest. Looking forward, we briefly discuss our on-going work on developing methods and codes for 3- and 4-particle correlated excitations which will address phenomena such as exciton-exciton interactions, formation of biexcitons and trions, decay of a single exciton into two excitons (fission), etc.