HL 3: Invited Talk Friedhelm Bechstedt

Time: Monday 9:30–10:00 Location: POT 081

Invited Talk HL 3.1 Mon 9:30 POT 081

Parameterfree calculations of excitations and spectra: Fiction or reality for semiconductors? — •Friedhelm Bechstedt — Friedrich-Schiller-Universitaet, Jena, Germany

The dream of theorists annd computational physicists is to have predictive power for important material properties and physical effects. Its realization requires ab initio calculations without experimental input parameters but accounting fully for the many-body interactions. The status of realization is examined for electronic excitations and related spectra. The basic approaches - density functional theory and many-body perturbation theory (quasiparticle and excitonic effects) - are introduced. Progress, accuracy problems, and applications are discussed for three classes of properties: (i) atomic equilibrium geometries, (ii) energies of electronic quasiparticles, and (iii) optical spectra including electron-hole pair excitations. Results are exemplarily presented for band structures and photoemission/X-ray/optical spectra of semiconductors such as Si, nitrides and oxides. The outlook concerns free carriers, defects, and nanostructures.