Understanding many-particle effects: accurate theories for liquids and electronic excited states in solids

Dr. Johannes C. Lischner
UC Berkeley/Lawrence Berkeley National Laboratory

Abstract:

The calculation of many properties of materials requires a detailed understanding of the interactions between the microscopic constituents. In my talk, I will first introduce a microscopically informed continuum theory which allows for an accurate and efficient modelling of interacting inhomogeneous molecular liquids, such as liquid water, and the description of solvation processes and liquid-solid interfaces. Then I will discuss accurate theories for electronic excited states. Specifically, I will demonstrate how the multiplet structure of quasiparticle excitations in magnetic defects, such as the negatively charged nitrogen-vacancy defect in diamond, can be calculated by means of GW theory. Finally, I will explain satellite features, which were observed in recent angle-resolved photoemission experiments on silicon and doped graphene, using the GW+cumulant theory for the electron-plasmon coupling.