CFEL SCIENCE

SEMINAR

5th August 2015 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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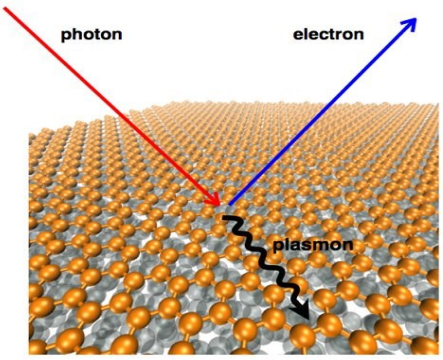
Theoretical Spectroscopy beyond GW

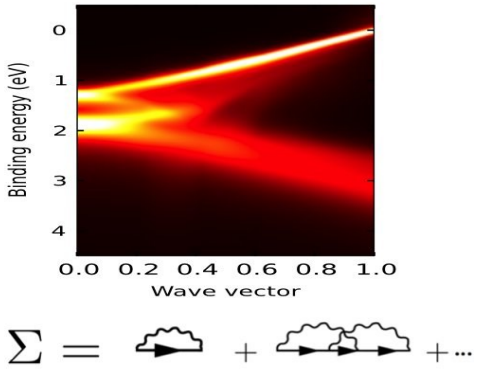
Spectral functions are measured in photoemission and tunneling experiments. The GW method is the state-of-the-art approach to calculate spectral functions that include many-electron interaction effects beyond density-functional theory. While GW theory has been very successful for the description of quasiparticle excitations in a wide range of physical systems including semiconductors and insulators, other systems and properties require going beyond the standard formalism.

For open-shell systems, such as magnetic molecules or magnetic defects in solids, I have developed a Green's function approach based on the GW approximation. In these systems, the poles of the self-energy give rise to the characteristic multiplet structure observed in photoemission experiments. For the calculation of plasmon satellite features in spectral functions, GW plus cumulant theory cures the failure of GW theory, which is known to significantly overestimate the separation of quasiparticle and satellite peaks. I will apply this method to silicon, doped graphene and the two-dimensional electron gas and demonstrate that it yields good agreement with experimental photoemission spectra. Finally, I will present a first-principles approach to include the coupling of quasiparticles to spin fluctuations, which play an important role in metals, magnets and unconventional superconductors.

a) photoemission experiment on doped graphene



b) computed spectrum and Feynman diagrams



Host: Angel Rubio – MPSD-CFEL Theory Department