INTERNSHIP PROPOSAL

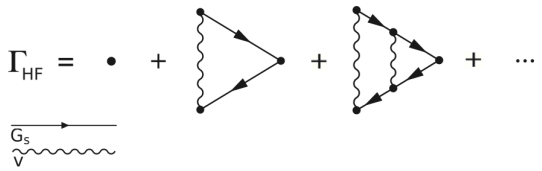
Title:

Effects of self-consistency on the quasiparticle spectrum within GW and beyond

Keywords: ab-initio simulations, diagrammatic techniques, RPA, GW, DFT

Scientific description:

The quasiparticle spectrum provides key information about new materials and can be theoretically analysed through the one-particle Green's function. The latter needs, however, to be approximated, including effects of the electron-electron interaction. In solids, any approximation should, e.g., incorporate screening, i.e., the collective electronic motion that weakens the long-range Coulomb interaction. Replacing the bare Coulomb interaction, v, in Hartree-Fock theory with the screened Coulomb interaction, W, leads to the GW approximation, known to provide a reasonable description on a wide range of systems. Although a unique GW solution exists in most cases, the high computational cost in practical calculations necessitates some additional approximation scheme (perturbative G_0W_0 with various starting points, GW with partial self-consistency or the so-called self-consistent quasiparticle GW). Unfortunately, the results often strongly depend on the chosen scheme. In this project we will study an alternative to these GW methods by combining it with the density functional formalism and the random phase approximation. In this way, a unique and self-consistent result is obtained. We will carefully assess the quality of the results on a number of solids and then formulate a beyond-GW method that, in addition to effects of screening, also captures excitonic effects.



References: *PHYSICAL REVIEW B **98**, 045117 (2018), PHYSICAL REVIEW B **103**, 075101 (2021)*

Techniques/methods in use: Many-body Green's functions, Density Functional Theory, Electronic structure codes (Quantum ESPRESSO, YAMBO)

Applicant skills: Background in solid-state physics. Mathematical skills. Basic programming skills.

Industrial partnership: N

Internship supervisor:

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Internship location:

Institut de Minéralogie, Physique des Matériaux et Cosmochimie (IMPMC), Equipe: TQM: http://www.impmc.upmc.fr/fr/equipes/ theorie_quantique_des_materiaux.html

Possibility for a Doctoral thesis: Y