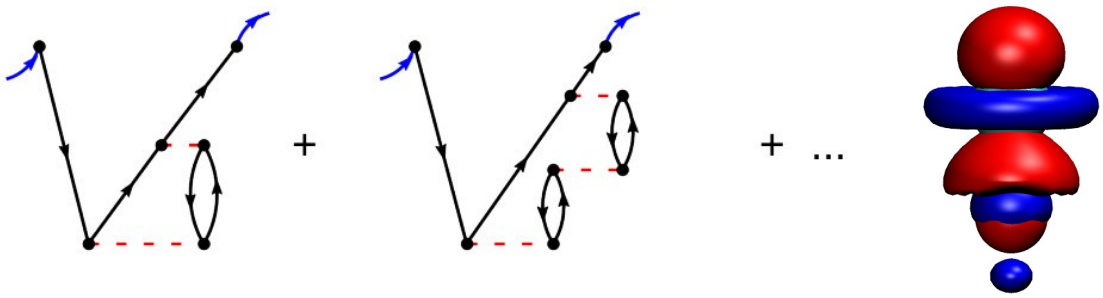
Post-doctoral position opening
CEA Saclay – Université Paris-Saclay
January 2020



Position

A one year (with a possible extension to 2 years) post-doctoral position is open at SRMP lab, CEA, Université Paris-Saclay, starting in early 2020. The post-doctoral fellow is to join a collaborative project “ABInit implementation of improved Density Matrix”, with Dr. Fabien Bruneval (CEA Saclay) and Dr. Marc Torrent (CEA Bruyères-le-Châtel), funded by the CEA cross-cutting program “Numerical Simulation”.

Scientific context and goals

The GW approximation to the electronic self-energy is most famous for predicting the correct band gaps of semiconductors and insulators [1,2]. However, we have shown very recently that the GW approxmation (obtained from Feynman diagrams) is also excellent for calculating the density matrix of molecules [3,4]. The density matrix gives access to many properties: the electronic density, the electrostatic potential, the kinetic energy, the NMR shielding, etc.

The main purpose of the project is to implement and then test the quality of the GW density matrix for condensed matter systems. The implementation will be based on the open-source code ABINIT [5,6], of which the two supervisors have been active developers for years. The expected outcome are improved electronic densities going beyond density-functional theory (DFT). We expect to predict improved electronic properties for realistic solid-state systems: surfaces, semi-conductor junctions, NMR shieldings in solids, etc.

Requested skills

We are looking for a skilled and motivated candidate who is proficient with solid state physics and computer programming. The candidate will have to interact with the two groups involved in the collaboration, as well as the ABINIT developer community.
Please send your application to both Fabien Bruneval and Marc Torrent with a complete CV including references that we may contact.

Contacts

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References

[1] *New Method for Calculating the One-Particle Green's Function with Application to the Electron-Gas Problem,* L. Hedin, Phys. Rev. **139**, A796 (1965).
[2] *The GW approximation: content, successes and limitations*, L. Reining, WIREs Comput. Mol. Sci. **8**, e1344 (2018).
[3] *Improved density matrices for accurate molecular ionization potentials*, F. Bruneval, Phys. Rev. B **99**, 041118(R) (2019)
[4] *Assessment of the linearized GW density matrix for molecules*, F. Bruneval, J. Chem. Theory Comput. **15**, 4069 (2019).
[5] http://www.abinit.org
[6] *Recent developments in the ABINIT software package*, X. Gonze *et al.,* Computer Physics Comm. **205**, 106 (2016).