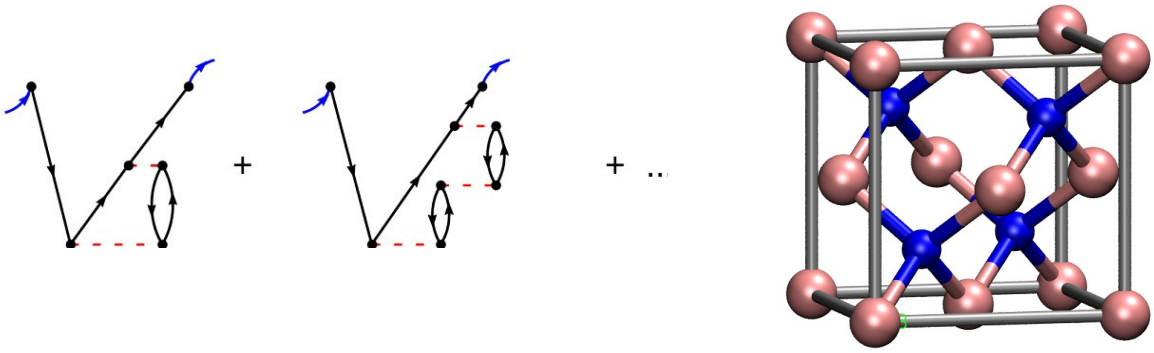
Post-doctoral position opening
CEA Paris Saclay / Université Paris-Saclay
January 2022



Position

A one year (with a possible extension to 2 years) post-doctoral position is now open at CEA Paris-Saclay / Université Paris-Saclay. The post-doctoral fellow is to join a collaborative project “ABInit implementation of improved Density Matrix”, with Dr. Marc Torrent (CEA Bruyères-le-Châtel) and Dr. Fabien Bruneval (CEA Saclay), 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 approximation (obtained from Feynman diagrams) is also excellent to calculate the density-matrix of molecules [3,4,5]. The density matrix gives access to many properties: the electronic density, the electrostatic potential, the kinetic energy, the NMR shielding, etc.

The GW density-matrix has been recently implemented in the open-source code ABINIT [6,7]. The main goal of this project is to quantify the performance of this new density-matrix for real materials. If the performance is confirmed, the GW density-matrix would constitute an very relevant alternative to density-functional theory.

Requested skills

We are looking for a skilled and motivated candidate who is proficient with solid-state physics and computer simulations. Coding skills would be appreciated. The candidate will have to

interact with the two groups involved in the collaboration, as well as the very active ABINIT developer community.

Please send your application to both Marc Torrent and Fabien Bruneval 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] *Improved One-Shot Total Energies from the Linearized GW Density Matrix,* F. Bruneval, M. Rodriguez-Mayorga, P. Rinke, M. Dvorak, J. Chem. Theory Comput. **17**, 2126 (2021).
[6] http://www.abinit.org
[7] The Abinit project: Impact, environment and recent developments, X. Gonze *et al.,* Computer Physics Comm. **248**, 107042 (2020).