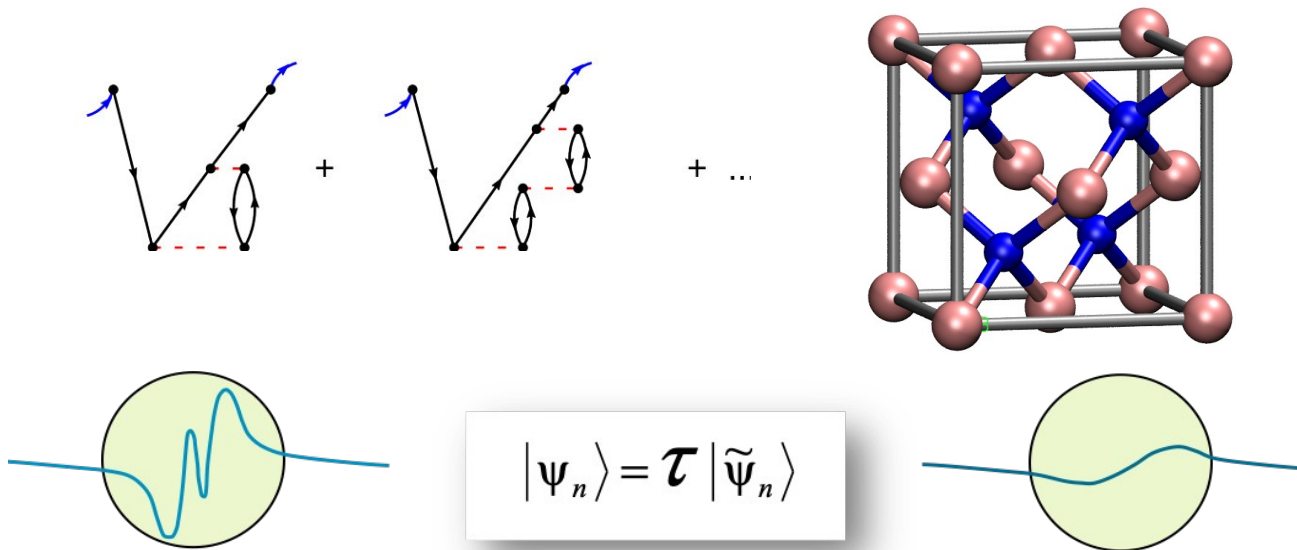




Post-doctoral position opening
CEA Bruyères-le-Châtel – CEA Saclay
Université Paris-Saclay
January 2021



Position

A one year (with a possible extension to 2 years) post-doctoral position is now open at CEA Bruyères-le-Châtel / 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 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 GW density matrix has been recently implemented in the open-source code ABINIT [5,6]. However, it is crucial for accuracy to employ the Projector Augmented Wave (PAW) method in this context [7,8]. PAW has an all-electron quality, but retaining the ease of use of regular

plane-wave basis. The inclusion of PAW technology will require sizeable code developments. The CEA group in Bruyères-le-Châtel has been leading the PAW developments in ABINIT for the last decade [9].

With the combined GW density-matrix and PAW technologies, 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 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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