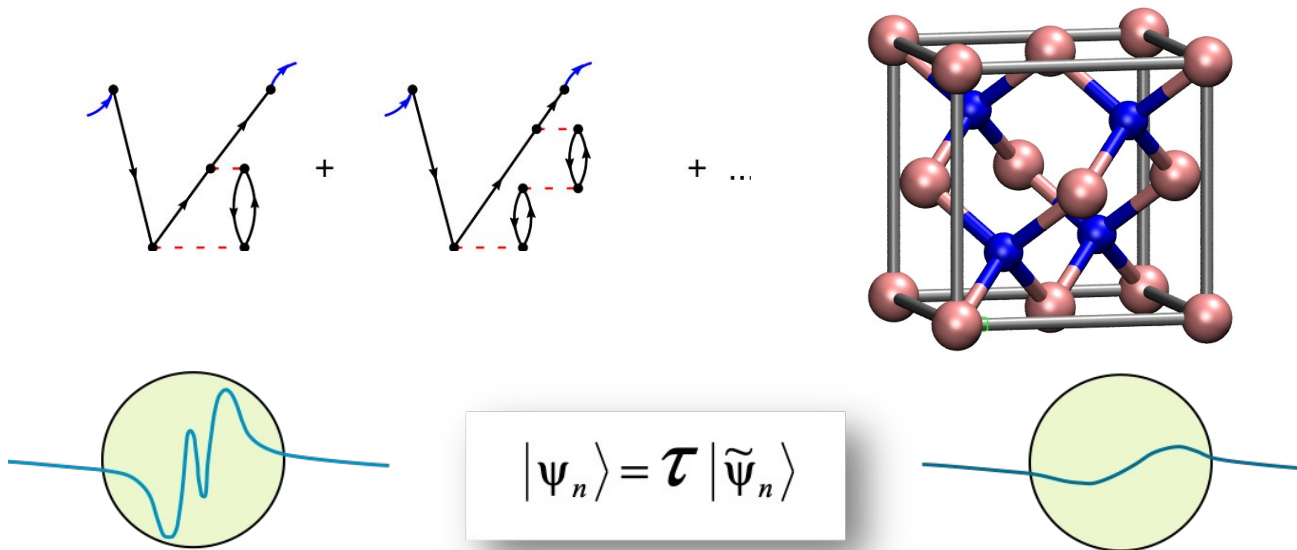




Post-doctoral position opening
CEA Bruyères-le-Châtel / CEA Saclay
Université Paris-Saclay
April 2021



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 conducted by 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 is a Feynman diagram technique for electronic structure, which has gained fame for predicting the correct band gaps of semiconductors and insulators [1] and the ABINIT software project [2] was certainly the first open-source code to include the GW calculations in its suite.

The Projector-Augmented Wave (PAW) [3] has triggered a revolution in the density-functional theory codes: it has boosted the precision [4] and speed. Indeed, PAW permits the correct description of the wavefunctions and of the effect of core electrons, while keeping the computational burden relatively low.

The hired postdoctoral fellow is to develop the robustness and speed of the current implementation of the PAW technology in the ABINIT-GW code. We aim at improving the precision and at adapting the code to modern high-performance computers.

Such developments will open up new applicative prospects for GW calculations in materials, with a special interest in getting correlated total energies and density-matrices [5].

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 other ABINIT developers.

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

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- [4] *Reproducibility in density functional theory calculations of solids*, K. Lejaeghere et al., Science **351**, 1410 (2016).
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