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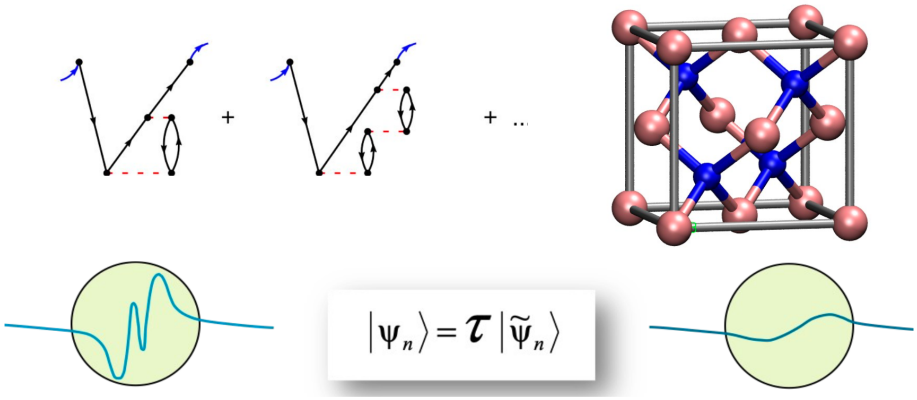

Excited electronic states calculations in the GW approximation coupled to the Projector Augmented-Wave Approach

Position

A 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 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 main goal of this project is to address a significant gap in the chain of ab initio calculations used to predict the microscopic properties of materials, specifically by enabling reliable calculations of excited electronic states (GW method) [1] within the Projector Augmented-Wave (PAW) approach [2]. These developments are intended for integration into ABINIT, a highly visible international open-source software project [3]. The GW approximation is recognized as the reference method for determining electronic energy levels in condensed matter, notably solving the well-known “band gap problem” of DFT, which typically underestimates the band gap with local or semi-local approximations. The PAW approach, which combines the advantages of pseudopotential methods with high precision regardless of electronic wavefunction shape, is widely used for ground-state calculations and material response. However, existing GW-PAW formalisms [4, 5], despite published theories, fail in certain well-identified cases (such as zinc oxide). While low-energy excited states are reasonably well described, high-energy states remain problematic. The current debate centers on whether to perform full (but computationally demanding) calculations, to neglect certain terms (with complex error control), or to modify the PAW method (at the cost of reduced efficiency) [6]. The broader objective of this project is to revisit these issues, adapt the PAW formalism to the GW approach, and develop a numerical scheme that is both

faster and more accurate than current methods, thereby clarifying and improving upon the present, somewhat confused, situation.
With the combined GW and PAW formalism, we expect to predict improved electronic properties for realistic solid-state systems : surfaces, semi-conductor junctions, etc.

The CEA team is one of the main driving forces behind the development of ABINIT, particularly regarding the PAW and GW approaches, as well as developments related to high-performance computing. Access to the CEA's significant computational resources will be ensured.
The objectives of the postdoctoral position combine both theoretical development and implementation : studying various pathways to resolve the reliability issues of GW calculations within the PAW approach, implementing the chosen solution(s) in the ABINIT software, computing improved electronic properties for realistic solid-state systems.

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.

In accordance with French legislation regarding postdoctoral contracts, the candidate's doctoral degree must have been obtained less than three years ago.

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] *The GW approximation : content, successes and limitations*, L. Reining, WIREs Comput. Mol. Sci. 8, e1344 (2018).

[2] *Projector augmented-wave method*, P. Blöchl, Phys. Rev. B 50, 17953 (1994)

[3] ABINIT web site : `www.abinit.org`

[4] *Implementation of an all-electron GW Approximation using the Projector Augmented Wave method*, B. Arnaud, M. Alouani, Phys. Rev. B 62, 4464 (2000)

[5] *Implementation and performance of the frequency-dependent GW method within the PAW framework*, M. Shishkin, G. Kresse, Phys. Rev. B 74, 035101 (2006)

[6] *Predictive GW calculations using plane waves and pseudopotentials*, J. Klimes, M. Kaltak, G. Kresse, Phys. Rev. B 90, 075125 (2014)