O.26 GW1RDM: the one-body reduced density-matrix from the *GW* approximation in ABINIT

Mauricio Rodriguez-Mayorga[1], Marc Torrent[2] and Fabien Bruneval[1]

[1] *Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*

[2] *CEA, DAM, DIF, F-91297 Arpajon, France, and Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, 91680 Bruyères-le-Châtel, France.*

The *GW* approximation is known for giving the correct band gap of semiconductors and insulators. However in principle, it allows one to obtain the electronic density and the density-matrix.

Guided by the nice results obtained recently for molecules [1,2], we have introduced the *GW* one-body reduced density-matrix in our favorite plane-wave code, ABINIT. With this implementation based on imaginary frequencies, we can calculate several interesting electronic properties:

- Electronic densities which are not DFT-based
- Density-matrix with fractional occupation numbers
- Kinetic energies that include the correlation part
- Total energies which are close to the self-consistent *GW* result

We examplify our implementation with a few semiconductors and insulators and compare with some very recent Quantum Monte-Carlo results [3].

---

[1] F. Bruneval, *Assessment of the Linearized GW Density Matrix for Molecules*, JCTC **15**, 4069 (2019).

[2] F. Bruneval, M. Rodriguez-Mayorga, P. Rinke, M. Dvorak, *Improved One-Shot Total Energies from the Linearized GW Density Matrix*, JCTC **17**, 2126 (2021).

[3] S. Chen, M. Motta, F. Ma, and S. Zhang, *Ab initio electronic density in solids by many-body plane-wave auxiliary-field quantum Monte Carlo calculations*, PRB **103**, 075138 (2021).