

Abstract Submitted  
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**MBPT calculations with ABINIT**<sup>1</sup> MATTEO GIANTOMASSI, Université catholique de Louvain, NAPS, Louvain-la-Neuve, Belgium, GEORG HUHS, Barcelona Supercomputing Center, DAVID WAROQUIERS, XAVIER GONZE, Université catholique de Louvain, NAPS, Louvain-la-Neuve, Belgium — Many-Body Perturbation Theory (MBPT) defines a rigorous framework for the description of excited-state properties based on the Green's function formalism. Within MBPT, one can calculate charged excitations using *e.g.* Hedin's *GW* approximation for the electron self-energy. In the same framework, neutral excitations are also well described through the solution of the Bethe-Salpeter equation (BSE). In this talk, we report on the recent developments concerning the parallelization of the MBPT algorithms available in the ABINIT code ([www.abinit.org](http://www.abinit.org)). In particular, we discuss how to improve the parallel efficiency thanks to a hybrid version that employs MPI for the coarse-grained parallelization and OpenMP (a de facto standard for parallel programming on shared memory architectures) for the fine-grained parallelization of the most CPU-intensive parts. Benchmark results obtained with the new implementation are discussed. Finally, we present results for the *GW* corrections of amorphous SiO<sub>2</sub> in the presence of defects and the BSE absorption spectrum.

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