Low-complexity MP2 for solids

Tobias Schäfer[a] and Georg Kresse[b]

[a] *Institute for Theoretical Physics, Vienna University of Technology* , [b] *Faculty of Physics, Center for Computational Materials Science, University of Vienna*
tobias.schaefer@mailbox.org

Hartree-Fock plus MP2 is a standard approach in materials physics and quantum chemistry to evaluate the energy of matter. However, this is computationally very demanding since conventional MP2 implementations scale with the fifth power of the system size, $O(N^5)$, and are difficult to parallelize. We present two low-complexity implementations that have a lower scaling and an almost ideal parallelization efficiency. The key concept of both approaches is to eliminate the summation over all combinations of occupied and unoccupied states, which can be elegantly achieved in the Laplace transformed MP2 formulation [1]. In this way we attain a quartic scaling high performance algorithm, $O(N^4)$, in the plane-wave basis without introducing further approximations. Moreover, using stochastic HF orbitals, a cubic scaling, $O(N^3)$, can be achieved when a fixed absolute error is assumed which turns into a linear scaling, O(N), when only a fixed relative error is assumed (e.g. per atom) [2, 3]. Analogously, the approaches could allow us to calculate second-order screened exchange as well as particle-hole ladder diagrams with a similar low complexity.

References

1. T.Schäfer, B. Ramberger, G. Kresse, J. Chem. Phys. 146, 104101 (2017).
2. T.Schäfer, B. Ramberger, G. Kresse, J. Chem. Phys. 148, 064103 (2018).
3. D. Neuhauser, E. Rabani, R. Baer, J. Chem. Theory Comput. 9, 24 (2013)