GW with Slater Type Orbitals

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I will talk about the implementation of the GW approximation in ADF[1]. After giving a short general introduction to the GW method, I will talk about the advantages of the implementation in ADF and present computational timings. I will also discuss the need for an extrapolation of quasi-particle energies to the complete basis set limit to obtain accurate results. To perform such a basis set limit extrapolation, we have designed new Slater Type basis sets for the whole periodic table. Using these basis sets, I will demonstrate that ADF give quasi-particle energies which are in good agreement with other implementations using plane-waves or Gaussian type orbitals as single-particle basis set.

1 Förster, A.; Visscher, L. Low-order scaling G_0W_0 by pair atomic density fitting J. *Chem. Theory Comput.* **2020**,16, 7381–7399.