An O(N^3) implementation of Hedin's scheme for molecules in organic semi conductors

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The improved scaling of our method with respect to most published methods is a step forward towards the goal of predicting, prior to their synthesis, the ionization energies and electron affinities of the large molecules that serve as constituents of organic semiconductors.

Here we focus on the principle of locality that previously lead to an efficient solution of the Petersilka-Gossmann-Gross equations of TDDFT and which gives rise to N^3 scaling with the number of atoms N in Hedin's approach for molecules.

For more details on our results, see the contribution by P. Koval on "O(N^3) GW" at the session on HPC.

References

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