



Introduction

Real-time time-dependent density functional theory (RT-TDDFT) [1] is a powerful tool for investigating time-dependent responses and electronic dynamics of molecules and materials. Back in 2020, I had the privilege of being part of a team that reported an implementation of RT-TDDFT using Gaussian-type orbitals, the Magnus propagator, and self-consistent field and predictor-corrector time integration schemes [2].

Notes about Implementation

The implementation of RT-TDDFT within the [TURBOMOLE](#) program package [3] uses Gaussian-type orbitals as basis functions along with second and fourth-order Magnus expansions. Time integration uses the self-consistent field as well as the predictor-corrector schemes. The Coulomb contribution to the Kohn–Sham matrix is calculated by combining density fitting approximation and the continuous fast multipole method.

Results

We benchmarked the implementation on molecular systems of different sizes and dimensionalities, including linear alkane chains. We found that the wall time for the density matrix time propagation step was comparable to the KS matrix construction.

Conclusion

This work contributes to the ongoing development of RT-TDDFT as a valuable tool for understanding electronic structure in a wide range of materials and molecules. The use of Gaussian-type orbitals in our implementation improves both accuracy and efficiency, while our method for calculating Coulomb contributions offers an additional way to accelerate RT-TDDFT calculations. Overall, I believe that this work will be useful to researchers in many fields who are interested in using RT-TDDFT to study electronic structures under external electric fields.

References

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