Quantum-chemical methods for calculating molecular response properties: low-, linear-, and sublinear-scaling methods

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The calculation of molecular response properties is a major challenge for very large systems with 1000 and more atoms. The talk will provide an overview of our low-, linear-, and sublinear-scaling response methods. Various quantum-chemical levels ranging from HF, DFT, MP2, to RPA will be discussed (e.g., Refs. [1-3]).

In addition, we introduce a novel semi-numerical integration scheme that allows for linear-scaling exchange-type contractions on both CPUs and GPUs leading to speedups of two to three orders of magnitude [4,5] as compared to conventional integration. This not only accelerates static calculations, but also ab-initio molecular dynamics simulations and the necessary sampling for complex systems.

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[3] M. Glasbrenner, D. Graf, C. Ochsenfeld,
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[4] H. Laqua, T. H. Thompson, J. Kussmann, C. Ochsenfeld,
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[5] H. Laqua, J. Kussmann, C. Ochsenfeld, J. Chem. Phys. 154, 214116 (2021).