Cost-Effective Treatment of Relativistic Effects

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Relativistic effects need to be considered in quantum-chemical calculations when dealing with heavy-element compounds or when aiming at high accuracy. In the latter case these effects are even important for systems containing only light elements. In order to allow a routine treatment of relativistic effects, cost-effective as well as accurate schemes are needed which in particular are also applicable in the context of electron-correlation calculations. Two approaches will be pursued for this purpose in the following:

- direct perturbation theory (DPT) with a special emphasis on higher-order treatments;
- spin-free approaches based on a non-perturbative treatment of the scalar-relativistic effects. Spin-orbit coupling is here treated afterwards using perturbation theory.

In the lecture, the theoretical background of these schemes is discussed, and results for energies and molecular properties are given to judge the accuracy of the presented schemes.