Relativistic Calculation of Magnetic Properties of Molecules

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In this talk I will consider the use of the 4-component Dirac equation in electronic structure calculations. Substituting the Schrdinger equation by the Dirac equation in quantum chemical methods provides an unique way of incorporating both scalar relativistic and spin-orbit effects in the calculation. It also gives rise to a number of interesting conceptual differences with non-relativistic theory. Two examples that will be discussed are the calculation and interpretation of spin-orbit effects and the calculation of the diamagnetic contributions to NMR parameters. We are now entering the stage where routine application of 4-components methods to molecular systems is only limited by the large computational resources required and the lack of efficient implementations for some of the post-Hartree-Fock methods. I will first discuss the computational scaling of the various 4-component methods in comparison with both non-relativistic and more approximate relativistic methods. After that I will give an overview of the strategies that can be followed to overcome the remaining computational bottlenecks. In the applications section I will focus mainly on the calculations of NMR parameters as these parameters are determined by the shape of the wave function near the nuclei and are hence heavily influenced by relativistic effects.