Séminaire de Chimie Théorique

Salle conference 3eme Est, Bat. A12
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(Some) Spectroscopy 'in Silico'

Molecular "response" properties are underlying virtually all spectroscopic and optical properties. They can be computed from first principles in form of derivatives of the energy (static properties) or the quasi-energy (dynamic properties), with suitable chosen derivative parameters such as electric and magnetic field amplitudes, nuclear spin magnetic moments, geometrical distortions, and others. We will give a brief overview of methods for calculating electric and magnetic response properties of molecules in the framework of density-functional theory (DFT), and discuss selected applications to organic molecules and transition metal complexes. Emphasis will be placed on computational studies employing recently developed modules in the open-source NWChem package for NMR and EPR calculations, and for calculations of electronic optical activity. An analysis of calculated molecular properties in terms of local atomic or orbital contributions may be used for the design of new materials or to help identifying shortcomings in approximate theoretical methods. Further, we will consider some specific shortcomings of DFT in molecular property calculations. An example is the electric field gradient at copper in the CuCl molecule. Most density functionals do not even predict the correct sign. Another example is the coupling of excitations in molecules with two or more spatially separated chromophores. We will discuss the reasons for these failures, and some ideas for systematically improving the calculations.

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