Molecular spectroscopy: Where theory meets experiment

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By considering the interactions between the molecular electronic structure and external electric and magnetic fields, as probed in a wide range of experimental spectroscopic techniques, a detailed understanding of the electronic structure of molecules can be obtained. Spectroscopy represents a direct link between the experimental observation of a molecule and electronic-structure calculations. By computing experimental spectra, including all possible effects, accurate, high-resolution experimental spectra can provide a very stringent test of the quality of a computational method and thus its description of the electronic structure of the molecule.

Simultaneously, theory can in many cases provide additional insight into the origin of experimentally observed spectra, assuming that we are able to calculate all the processes and interactions that are involved in the experimental measurement. Together, theoretical and computational spectroscopy can provide unique and detailed insight into the molecular responses to electromagnetic field.

In this talk, I will outline the principles for calculating molecular properties for any element of the periodic table. A particular focus will be on the calculation of the nuclear magnetic shielding constants of nuclear magnetic resonance (NMR) spectroscopy, which describes the coupling between the nuclear magnetic moment and an external magnetic field. I will in particular focus on the use of NMR to determine absolute shielding constants and nuclear magnetic dipole moments.

If time allows, I will also give some recent examples from our work on multiphoton spectroscopy both in the electronic and vibrational frequency range.