Nonlinear chiroptical properties and spectroscopies

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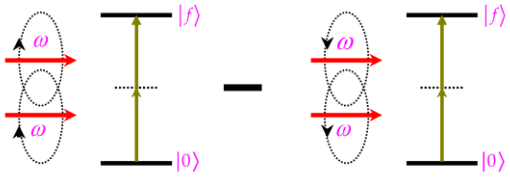
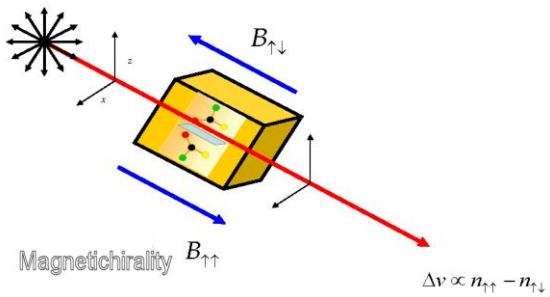
In this talk the speaker will review the latest developments in the theoretical and computational studies of nonlinear optical properties and spectroscopies involving the concept of chirality.

The results of a combined experimental-computational analysis of the two-photon circular dichroism of some bi-aryls (BINOL, VANOL, VAPOL) exhibiting structural chirality will presented. The challenges faced in the *ab initio* calculation of nonlinear optical properties in molecules of the size and complexity of those mentioned just above will be discussed. They involve the careful choice of appropriate basis sets, electronic structure and condensed phase models, besides the need to account properly for the effect of molecular vibrations, conformational variety and magnetic gauge origin invariance [1].



The focus will then shift to other nonlinear spectroscopic properties, proven to be amenable to ab initio simulation resorting to the tools of modern analytical response theory: excited state electronic circular dichroism, circular intensity difference arising in second harmonic generation and a general family of birefringences and dichroisms arising in the interaction of radiation with chiral samples [2]. Special emphasis will be on the phenomenon of magnetochirality, the axial birefringence and the related dichroism observed when an unpolarized light beam interacts with chiral sample in the presence of a magnetic field with a component parallel to the direction of propagation [3].



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[3] B. Jansík, A. Rizzo, L. Frediani, K. Ruud, S. Coriani J. Chem. Phys. (2006), 125, 234105