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"COMPUTATION OF VIBRATIONAL CIRCULAR DICHROISM IN THE CONDENSED PHASE: AN INTERPLAY OF STRUCTURE AND DYNAMICS"

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ABSTRACT

Chiroptical spectroscopy provides an increasingly important, cost-effective alternative for the study of chiral substances. In recent years, vibrational circular dichroism (VCD) – the chiral form of IR absorption spectroscopy – has come into focus as a very sensitive probe of molecular conformation and environment. It has been applied to a wide range of molecules including natural products, host-guest systems, proteins, nanoparticles, or catalysts, as well as the formation of chiral phases from achiral subunits. VCD differs from electronic circular dichroism in that it relates directly to vibrational transitions in the supramolecular chiral framework, such as functional groups connected by covalent or non-covalent interactions (hydrogen bonds etc.).

Accurate calculations are required to interpret VCD spectra, but unlike conventional IR absorption spectroscopy, they cannot be performed within the Born-Oppenheimer approximation. Nowadays, these properties are determined using linear quantum response theory and have become a standard feature of many quantum chemical codes. However, the vibrational analysis of large systems can be challenging and requires a special treatment of the conformational freedom and large amplitude motions. Therefore, instead of working with optimised geometries and within a static picture, we deploy molecular dynamics simulations in order to obtain a realistic image of the molecular conformers and the anharmonic coupling of vibrational modes in the condensed phase.

This talk discusses the origins of non-local VCD patterns that emerge in supramolecular aggregates, which we can analyze and understand in detail using our theoretical tools. Our results emphasize the capabilities of VCD spectroscopy for chiral structure determination and its susceptibility for supramolecular symmetry.