Minicolloque n° 26 [X] **Oral** [ ] **Poster**

Chiroptical and magnetic properties of lanthanide complexes from an *ab initio* point of view

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There is a growing interest in the use of circular dichroism (CD) and circularly polarized luminescence (CPL) for the structural characterization of chiral lanthanide-based complexes. Indeed, the sensitivity of these effects to the configurational and conformational environment around the lanthanide center enables to study structural changes in biological systems [1], as well as, to develop electroluminescent [2] or security [3] devices. However, the interpretation of CD and CPL spectra of such systems is by far not straightforward.

In the same time, since the pioneering work of van Vleck [4], it is well established that crystal field splitting is at the origin of both the magnetic and luminescent properties in lanthanide-based complexes. Consequently, both properties are strongly correlated and can be looked alongside. Magneto-chiral dichroism (MChD) is for instance one possible manifestation of this correlation [5].

In every instance, lanthanide-based complexes are very challenging for quantum chemistry due to (i) the presence of degenerate electronic states with multi-configurational character and (ii) the importance of the spin-orbit coupling in the calculations of the spin forbidden transitions [6]. Recent *ab initio* results over these topics, mainly focused on CD and CPL parameters, will be presented.

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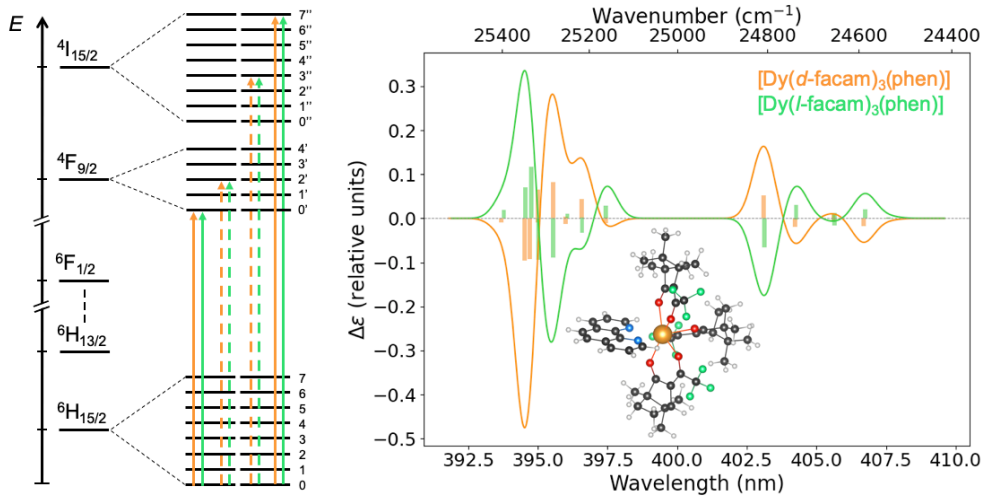

Figure 1. Simulated CD spectrum of the [Dy(*d*/*l*-facam)$_3$(phen)] complex (DFT ZORA-PBE0/TZP optimized structure) from CAS(9,7)SCF calculations.