Study of dynamical observables involved in photoionization process

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My talk will be focused on the study of dynamical observables which are involved in photoionization process for several systems.
We studied valence ionization of a coordination complex, with particular attention to the dichroic parameter profiles. These observables characterize chiral systems and can be used as "fingerprints" of the conformers. The computational approach, based on accurate solution of the scattering problem in a Density Functional framework, utilizes a discretization of both bound and continuum functions in a multicenter basis of B-spline functions times spherical harmonics [1].

We also developed a new method based on the use of Dyson orbitals for the correlated description of photoionization observables [2]. Correlated Dyson orbitals are particularly important for ionization of electronically excited states and of open-shell species, but relatively scarce procedures exist to determine them within high level ab initio approaches. Our aim is implementing ground and excited state Dyson orbitals for all members of the Coupled Cluster hierarchy, and coupling them to an efficient multicenter B-spline DFT code for the photoelectron. This scheme can be applied to investigate photoelectron processes and signatures where electron correlation plays a fundamental role, as for instance the valence inner-shell satellite bands of several gas-phase molecules and the core-ionization photoelectron spectra of heterocylic aromatic organic compounds.

[1] M. Stener, G. Fronzoni and P. Decleva, *J. Chem. Phys.,* 122, 2005

[2] A. Ponzi, C. Angeli, R. Cimiraglia, S. Coriani and P. Decleva, *J. Chem. Phys.*, 140, 2014