PhD GRANTS 2024

PhD project title: Novel electronic structure methods to simulate single and multiphoton excitation processes in chiral molecular systems

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PhD project summary (max. 20 lines):

The interaction between light and matter is key to understanding of physical processes taking place at the microscopic scale, as light acts as a probe to the electronic structure of atoms and molecules, in linear (involving one photon, such as in absorption, fluorescence etc.) or non-linear (involving two or more photons, such as second harmonic generation, two-photon absorption etc.) processes. In recent years, light-matter interaction has been applied to understand so-called chiral systems, as these have shown promise for chiroptoelectronic properties [1]. The chirality in such systems can be intrinsic, with molecules being themselves chiral, or arise through the interaction of non-chiral molecules with chiral environments. An understanting of the molecular origin of chiroptical properties can be gainded through theoretical modeling. That requires theoretical tools which are capable of accurately describing electron correlation and environment effects on the electronic structure of such (supra)molecular structures themselves and their interaction with light. Furthermore, in systems of such as perovskites, which contain heavy elements such as lead and iodine, such models must also take into account relativistic effects [2]. This project aims to develop novel methods and computational tools, capable of accounting for all of these effects, in the simulation of single and multi-photon excitation processes in chiral molecules or achiral molecules in chiral environments. These developments will be carried out as part of our ongoing developments in relativistic electronic structure [3] and quantum embedding methods [4].

References

[1] G Long et al, *Nature Reviews Materials*, **5**, 423 (2020)

[2] P Schwerdtfeger, OR Smits, P Pyykkö, *Nature Reviews Chemistry* 4, 359 (2020)
[3] X Yuan, L Halbert, L Visscher, ASP Gomes, *J Chem Theory Comput.* (2023). arXiv:2309.07295 [4] M De Santis et al, *J Chem Theory Comput.* **18**, 5992 (2022)