Post Hartree-Fock modeling of a metal-phosphonate

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This training period is proposed in the context of a Labex EMC3 project titled Rare-Earth Less Hybrid Materials with Exacerbated Lighting Characteristics (in french, abbreviated to MAHYTER).

Rare-earth are very widely used in current state of the art technologies. Despite the fact that they aren't rare, large demand on rare-earth supply has, and will likely, lead to crisis on the rare-earth market. That's why materials showing equivalent properties to rare-earth compounds — lighting, stability, and so on — are seek for. Among the would be candidate, metal oxide frameworks (MOF), are under intense investigation (about 5 international publication per day on this matter). Some of them exhibit very interesting properties, like aggregation-induced emission (AIE), or even exacerbated induced emission (AEE). Understanding those properties is a key challenge in modelling physics, that may help improve our capacity to intelligently designe new MOF based materials.

At the simulation level[1], the most widely used method for structure characterisation of those compound is density functional theory (DFT) ; while time-dependent density functional theory (TDDFT) and the family of post-DFT methods are used to some extent in order to study the emitting properties of those materials. The properties of those systems

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[1]cf. 'Computational characterization and prediction of metal-organic framework properties' by F.-X. Coudert and A.H. Fuchs, in Coord. Chem. Rev. 2015 (DOI:10.1016/j.ccr.2015.08.001) for a review paper.

are stretching the current simulation capacities to their extreme limits. For the MAHYTER project we propose to investigate the possibility to study MOF optical properties based on post Hartree-Fock methods. Those methods are expected to yield much better insight on the excited states properties, yet it is currently unknown if it will be possible to tackle the problem with them.

The MAHYTER project is specifically targeted at studying the family of metal-phosphonates compounds. And so the training period work will be based on one of the simplest such compound.

Work: The study, will start by finding a stable structure of a compound, then studying the possibility to assess efficiently its electronic structure and resulting properties within the framework of Post-Hartree Fock methods. Performing this work will lead the trainee to get sensible skills in electronic structure computations.