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Pr Ria BROER
Université de Groningen, Pays-Bas - Zernike Institute for Advanced Materials, Un. of Groningen, The Netherlands - e-mail: r.broer@rug.nl

"The effects of electron correlation and relativity on the mechanisms of spin crossover in Fe(II) complexes"

The inclusion of the effects of electron correlation and relativity may complicate accurate quantum chemical study of molecules and materials, but on the other hand accounting for these effects is necessary for the design of materials with fine-tuned physical properties. This presentation discusses our recent quantum theoretical studies of the mechanisms of spin crossover in Fe(II) complexes. In these studies density functional theory, DFT, is combined with wave function based quantum chemical methods. Spin crossover can occur in complexes of transition metals with organic groups that induce a weak ligand field. The complexes have two low-energy spin states, and a transition between them can be induced by changing temperature, pressure or by light. Especially light-induced excited spin-state trapping, LIESST, is of technological importance. The crossover mechanisms may involve various processes like intersystem crossings and internal conversions. DFT gives us access to the equilibrium geometries and vibrational frequencies of the spin crossover complexes, while complete active space second order perturbation theory, CASPT2, reasonably describes the relative energies of the relevant spin states. This quantum chemical approach is combined with a time-dependent formalism for calculating intersystem crossing transition rates to elucidate the mechanism of the LIESST process. Our method allows us to reproduce the experimental time frame of the process and sheds light on the intermediate steps.

Contact : nicolas.galland@univ-nantes.fr – 02 51 12 55 71