SEMINAIRE ISMO

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Excited-state mechanisms and dynamics of the ruthenium nitrosyl complex trans-$[RuCl(NO)(Py)_4]^{2+}$

During the last three years of my PhD, I carried out a series of theoretical studies on the photochemistry of the ruthenium nitrosyl complex trans-$[RuCl(NO)(Py)_4]^{2+}$. In particular, in the first part of my talk, I will present the results of accurate ab initio calculations such as CASSCF/CASPT2, that shed light on the role of the excited states, highlighting the possibility of several photoisomerization pathways for the trans-$[RuCl(NO)(Py)_4]^{2+}$. The main IC and ISC pathways will be discussed, along with the spin-orbit couplings responsible for the ISC transitions. In the second part I will present the results of the full dimensional surface hopping dynamics on the same ruthenium nitrosyl complex, including the description of non-adiabatic and spin-orbit couplings. These results will confirm the assumptions of the ab-initio calculations. I will present an accurate estimation of the branching ratio between the different photoisomerization pathways, together with the identification of the most important quenching funnels that slow down the entire N→O isomerization process.

Mardi 12 mars 2019 à 11 h
Amphithéâtre du bât 520 (3ème étage)
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