Séminaire du laboratoire de Chimie Physique

JEUDI 3 NOVEMBRE 2016 à 11h00, salle Magat, bât. 349

"Towards in Silico Photochemical Experiments with Ab Initio Multiple Spawning"
par Basile Curchod (University of Bristol, UK)

What happens to a molecule once it has absorbed UV or visible light? How does the molecule release or convert the extra-energy it just received? Answering these questions clearly goes beyond a pure theoretical curiosity, as photochemical and photophysical processes are central for numerous domains like energy conversion and storage, radiation damages in DNA, or atmospheric chemistry, to name a few.

Ab initio multiple spawning (AIMS) is a theoretical tool that aims at an accurate yet efficient in silico description of photochemical and photophysical processes in molecules. AIMS describes the excited-state dynamics of nuclear wavepackets using adaptive linear combinations of frozen Gaussians. In this talk, I intend to survey some recent developments and applications of the AIMS technique.

An important feature of the AIMS formalism is its flexibility, which permits the addition of critical effects for a realistic simulation of photochemical processes. We for example recently included in AIMS spin-orbit coupling[1] and the effect of an external electric field[2], leading to two new schemes called Generalized AIMS (GAIMS) and eXternal Field AIMS (XFAIMS). We also proposed a simple yet rational approximation to AIMS termed Stochastic-Selection AIMS (SSAIMS), which allows decreasing the computational cost of an AIMS dynamics substantially[3].

To study the excited-state dynamics of large molecules, we also recently interfaced AIMS with the GPU-based electronic structure code TeraChem. Combining the accuracy of AIMS with the efficiency of GPU-accelerated electronic structure calculations (LR-TDDFT or SA-CASSCF) allows indeed for a significant step forward in the simulation of nonadiabatic events, as it pushes the boundaries of the well-known compromise between efficiency and accuracy imposed by the computational cost of such dynamics. Thanks to this new interface, we could investigate the nonadiabatic dynamics of different medium-size organic molecules important in biological chemistry[4,5], organic electronics[6], and atmospheric chemistry.


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