Nantes Université

Proposition de Stage Master CMT

Stage de M1 ☒ et/ou Stage de M2 ☒

Titre du stage : Reference potential energy surfaces for photochemistry

Equipe d'accueil : Modes/CEISAM

Responsable du stage :

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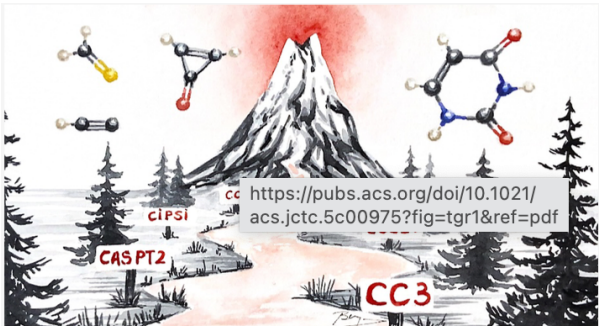
Description du stage proposé :

General framework

The accurate modeling of excited-state properties with *ab initio* quantum chemistry methods is a clear ambition of the electronic structure theory community that will certainly keep theoreticians busy for (at the very least) the next few decades. Beyond the access to accurate excitation energies, it is also important to explore potential energy surfaces (PES) since these are directly related to photochemical processes. The factors that make this quest for high accuracy PES particularly delicate are very diverse, but the theoreticians have now at hand a large panel of theoretical models to tackle these problems. A problem remains: how to produce reference values that can be used to benchmark "efficient" methods ?

Workplan

During this internship, the student will first use a large panel of coupled-cluster (CC) methods to define near-exact potential energy surfaces of a series of diatomics. Indeed this mono-dimensional problem remains challenging for theory, allows treating numerous states, and permits easy comparisons with experiment. The task will include identifying the key states, characterizing their nature, and computing their relative energies with various CC approaches and basis sets. In a second stage, the twisting of the ethylene will be considered, a prototype problem for *trans-cis* isomerization. In a third step, a series of less demanding methods, such as TD-DFT will be assessed using the reference data defined in the first step.



Key objectives

The key objectives will be to

1. Determine highly-accurate reference values with high-level CC methods for a series of model photochemical reactions.
2. Assess the performances of lower-order methods thanks to the reference values.

Expertise

The group has an extensive expertise in the techniques to be applied and used them often. The group in Nantes is the author of the QUEST database, the largest set of reference values for excited-state calculations. This set serves as the current reference worldwide.

Methods

During the internship, the student will use *ab initio* methods based on density functional theory (DFT) and wavefunction theories, implemented in programs available in the team. Prior expertise in the field is not necessary; this internship being oriented towards modeling aspects (use not developments).

Collaborations

The group collaborates with Drs. P.F. Loos and M. Boggio-Pasqua (Toulouse) on this topic. The internship is supported by the CARES ANR, led by Pr. D. Jacquemin.

Reference

The group has recently published a review-like paper on QUEST, see *J. Chem. Theory. Comput.* **2025**, *21*, 8010-8033.

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