

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Theoretical Chemistry

Title: DEVELOPMENT AND APPLICATION OF DENSITY BASED INDEXES FOR THE DIAGNOSTIC AND DESCRIPTION OF EXCITED STATES

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Ilaria Ciofini and Carlo Adamo

Advisor(s) Email: ilaria.ciofini@chimieparistech.psl.eu and carlo.adamo@chimieparistech.psl.eu

Research group/Lab: CTM group; i-CLeHS

Lab location: Institute of Chemistry for Health and Life sciences (i-CLeHS)
ChimieParisTech 11 rue P et M Curie, Paris

Website: <https://www.quanthic.fr/> **Twitter** https://twitter.com/group_ctm

Short description of possible research topics for a PhD:

In the last years our group has developed several indexes enabling both the description of the excited states in terms of their nature (Locally Excited vs Charge Transfer) and the diagnostic of problematic cases to be treated at DFT level. These descriptors have allowed the investigation of excited state Potential Energy Surfaces of relevance to disclose the photophysical properties and the photoreactivity of molecular systems of interest in difference fields ranging from photovoltaics, to health sciences (ex. photodynamic therapy).

Within this doctoral work we aim at developing new indexes allowing to follow excited state evolution and to apply them to rationalize and predict the behavior of photo-active molecules. Homogeneous photo-catalytic reactions will be the target in terms of application.

Required background of the student: The student should have a strong background in physical and theoretical chemistry. Previous knowledge in ab-initio methods and Density Functional Theory as well programming experience will be greatly appreciated.

A list of 5 representative publications of the group in the field :

1. JCTC 7 (2011) 2498-2506
2. COORD. CHEM. REV. (2015) 304-305 166-178
3. JCTC 16 (2020) 4543-4553
4. JACS 142 (2020) 6578-6587
5. Nature Comm 11 (2020) 3262.