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CALL FOR APPLICATIONS 2025 – FELLOWS

Supervisor	Emilie-Laure Zins
Supervisor page	https://www.researchgate.net/profile/Emilie-Laure-Zins-2
Host Institution	Sorbonne Université https://www.sorbonne-universite.fr/en
Research Lab	De la Molécule aux Nano-objets : Réactivité, Interactions et Spectroscopies https://www.monaris.cnrs.fr/
Research Team	Modélisation et Chimie Théorique https://www.monaris.cnrs.fr/2-mc2/

Project Title

Theoretical study of chemical bond modification and reactivity under physicochemical constraint

Project Description

Experimentally, molecules can be subjected to various types of physico-chemical constraints: electric field, chemical confinement .... These can affect, to a greater or lesser extent, the distribution of electron density within molecules, and hence their reactivity. To correctly describe these systems, and to be able to predict the evolution of reactivity as a function of stress, the main challenges consist in proposing specific descriptors based on the electronic structure of the molecule.

Keywords

ab initio calculations, topological analysis of electron density, characterization of chemical bonds

Description of the Host Research Lab

The laboratory's research activities are built on an approach shared by the different teams, based on the development, understanding and characterization, both experimental and theoretical, of nanophase systems, and in particular of chemical bonding in the construction of the organization and reactivity of matter.

To submit your application, please send an email with the required documents to msca-pf@sorbonne-universite.fr