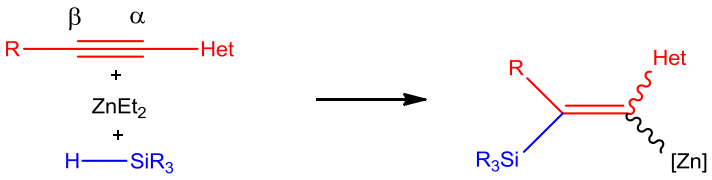
Post-doctoral Position

Unraveling the competition between Polar and RadIcal reactivity of Zinc rEagents: from computational modeling to synthetic methodology.

A 1 year post-doctoral position is available at Sorbonne University in Laboratoire de Chimie Théorique (LCT) in the area of *computational chemistry*. The position is funded by Labex MiChem. Salary will be around 2000 € per month (depending on working experience). Candidates are advised to apply as early as possible. The selection process will start immediately. The contract shall begin in October-December 2018.

The goal of this project is the determination of the reaction pathways in silyl- and germanylzincation of alkyne starting from sillylane (see below) or germane and diethyl zinc. Polar and radical mechanisms will be examined, as regio- and stereoselectivities are proposed to derive from a competition between these these two families of processes. Results will be compared to the available experimental data.



The DFT method will be used in a way to be appropriate for a large variety of electronic changes (involving both close and open shell systems, neutral and charges systems). Modeling of the complex reaction medium, in particular the solvation effects, will be considered as the system-environment interactions are expected to be different and play different roles for polar and radical mechanisms.

Collaboration: This work will be in collaboration with experimentalists (Dr. Pérez-Luna *et al.* Institut Parisien De Chimie Moléculaire, Sorbonne University). Solid experimental data are already available and the study will be carried out in parallel to an experimental PhD.

Qualifications: The candidate should have a PhD in Theoretical-Chemistry and an expertise in theoretical investigations of reaction mechanisms, preferably in organometallic chemistry. A good experience in the application of theoretical methods (DFT) for studying electronic and bonding properties of molecules will be appreciated. The candidate should additionally be very enthusiastic to interact with experimentalists and exhibit good pedagogical skills in this perspective. The postdoctoral fellow will use Density Functional Theory methods (Gaussian, ADF programs, …) as well as hybrid ONIOM or other QM/MM methods. Experience in computation of electronic structure of open-shell systems will be a significant advantage.

Interest candidates should send their CV, list of publications, cover letter and contact references by e-mail.

Laboratory: Laboratoire de Chimie Théorique UMR 7616 UPMC/CNRS – Tours 12/13 - 4, place Jussieu 75252 Paris - http://www.lct.jussieu.fr/

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