Post-doctoral position in Computational Chemistry and Catalysis (ICMUB – University of Burgundy)

Duration: 12 months extendable
Start date: ASAP (could be discussed)

Interested applicants should send a CV, a cover letter outlining their skill set and their research and career goals, and the contact details for two academic references.
Please submit the requested information by e-mail to: **Paul.Fleurat-Lessard@u-bourgogne.fr**

A postdoctoral position in Computational Chemistry is available in the group of Pr. Paul Fleurat-Lessard (http://pfleurat.free.fr/index.php) in Dijon at the Institut de Chimie Moléculaire (http://www.icmub.com/en/) in the Bourgogne Franche Comté University (France). The successful candidate will apply **electronic structure theory, DFT methods to investigate organometallic chemistry and catalysis mechanism.**

More specifically, this project corresponds to the theoretical study associated to the ALCATRAS ANR.
The ALCATRAS project is a fundamental research project aimed at developing innovative catalytic tools for C–H functionalization of heteroaromatics in cooperation with Dijon catalysis group (J.-C. Hierso).

The aim of the **post-doctoral project** is to help designing new ligands for new selectivity in CH activation. For this, we will analyse the electronic structure of the ligands and catalysts with AIM, ELF and NCI approaches to find chemical descriptors of the target reactions.[1,2]
In parallel, we will also study the mechanism of the CH activation using our home code to find the transition states.[3,4]

Requirements

- PhD in theoretical or computational chemistry or physics
- some knowledge of organometallic chemistry (especially with palladium)
- Be a curious and self-driven person
- Experience in mechanistic studies
- Some programming skills would be a plus.

Interested applicants should send a cover letter outlining their skill set and their research and career goals, a CV, and the contact details for two academic references.
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[1] Dalton Transactions, **2018**, *47*, 11203-11218. doi:10.1039/C8DT02364F
[2] Inorg. Chem. **2016**, *55*, 10907-10921. doi:10.1021/acs.inorgchem.6b01318
[3] Adv. Synth. Catal. **2019**, *361*,151 - 159. doi:10.1002/adsc.201801225
[4] ACS Catalysis **2018**, *8*,3067–3075. doi:10.1021/acscatal.8b00544;
ACS Catal. **2017**, *7*, 8493–8501. doi:10.1021/acscatal.7b03186