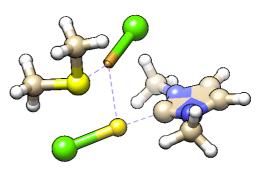
Postdoctoral Position at Aix-Marseille University

P. Nava & S. Humbel at the « Institut des Sciences Moléculaires de Marseille (iSm2)», invites applications for a postdoc position starting in winter 2021-2022.

The topic is about a computational design of transition metal catalysts bearing carbene ligands, notably N-heterocyclic carbene (NHC), containing a sole axial chirality. The position is financed by the French Research National Agency (ANR), within a project in close partnership with experimentalists.[1,2] Our target is the computational design of ligands to achieve configurationally stable complexes, through calculations of atropo-isomerism (barriers). Moreover, the mechanisms of transmetallation processes will be addressed too, in order to identify the crucial elements that might guarantee the chirality transfer.

Some incursions might be done to unveil catalytic mechanisms and understand how the catalyst's chirality can be transferred in model reactions. Prior experiences with first principles calculations, using quantum chemistry programs (notably DFT) are necessary. The position requires collaborative skills to work with experimentalists. as well as with other theoreticians. Very motivated candidates with a degree from physics, chemistry, materials science or related fields are encouraged to apply.



Applicants should use the CNRS website (offer: https://bit.ly/30WeASs.)

[1] L. Kong et al. J. Am. Chem. Soc 2020 142, 93[2] L. Kong et al. Adv. Synth. Catal. 2021, 363, 4229

Technical Details :

Full www address of the CNRS offer https://emploi.cnrs.fr/Offres/CDD/UMR7313-STEHUM-001/Default.aspx?lang=EN

Salary:

2750 - 3900 € /month depending on experience. => brut salary, including standard medical care.



Location:

The lab is in service 561, Campus St Jérôme, Marseille North. It possesses a significant computing facility (about 600 cores on its own + an access to the campus nodes). Due to the COVID, part of the work might be done in teleworking. Marseille is situated in France, on the Mediterranean coast and has a large national park "Les Calanques" where hiking is possible with outstanding panorama.