UMR 5254

Post-doctoral Position at UPPA, Pau, France. Understanding of reactivity of boron-nitrogen containing heterocycles by computational studies

12 months of post-doctoral position is available at the University of Pau at IPREM in the area of computational chemistry. The research will be carried out in collaboration with the group of Prof. Shih-Yuan Liu from Boston College. Salary will be around 2300 € per month, and this project is funded by I-SITE, E2S-UPPA (https://e2s-uppa.eu/en/jobs.html). In addition to research work, the contract involves 64 hours of teaching per year. Candidates are advised to apply as early as possible. The contract will begin in October 2019.

The project concerns the development of boron-nitrogen heterocycles and their potential utility as synthetic reagents and optoelectronic materials.

The relation between structure and electronic, spectroscopic and optical properties of these new compounds will be investigated by computational chemistry. Calculations will be mainly performed using Density Functional Theory (Gaussian, ADF programs…). Particular attention will be focused on the understanding/description of new catalytic transformations involving metal transition complexes with these boron-nitrogen heterocycles as ligands. Mechanistic studies (homogenous catalysis) will be carried out in order to anticipate or rationalize reactivity.

Qualifications : The candidate should have a PhD in Physical-Chemistry and a strong experience in the application of theoretical methods for studying electronic and optical properties. Strong expertise in the theoretical investigation of reaction mechanisms is required, with a major part of the experience being focused on the description of reaction pathways. The postdoctoral fellow will mainly use DFT methods (Gaussian, ADF programs,…). Knowledge of ONIOM, QM/MM methods will be appreciated. The candidate should be very enthusiastic and should appreciate to work on a collaborative experimental-theoretical project.

Laboratory : Institut des Sciences Analytiques et de Physico-Chimie pour l'Environnement et les Matériaux (IPREM, UMR 5254). Hélioparc 2 avenue P. Angot, 64053 Pau cedex 09 (France).

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Please send CV + motivation letter + recommendations.

Keywords : DFT – Electronic/optical properties - Energy profiles - Homogeneous catalysis.

Some references :

1- The Least Stable Isomer of BN Naphthalene: Toward Predictive Trends for the Optoelectronic Properties of BN Acenes. Z. Liu, J. Ishibashi, C. Darrigan, A. Dargelos, A. Chrostowska, B. Li, M. Vasiliu, D. Dixon, S-Y Liu. ***J. Am. Chem. Soc.***, **2017**, *139 (17)*, 6082.

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3- Catalytic Dehydrogenation of (Di)Amine-Boranes with a Geometrically Constrained Phosphine-Borane Lewis Pair. M. Boudjelel, E. D. Sosa Carrizo, S. Mallet−Ladeira, S. Massou, K. Miqueu, G. Bouhadir, D. Bourissou. ***ACS Catalysis***, *8*, **2018**, 4459.

4- A Stable but Highly Reactive Phosphine-Coordinated Borenium: Metal-free Dihydrogen Activation and Alkyne 1,2-Carboboration. M. Devillard, R. Brousses, K. Miqueu, G. Bouhadir, D. Bourissou, ***Ang. Chem. Int. Ed. Engl.***, *54*, **2015**, 5722.

5- Cyclometalated Gold(III) Complexes: Noticeable Differences between (N,C) and (P,C) Ligands in Migratory Insertion. J. Serra, P. Font, E. D. Sosa Carrizo, S. Mallet-Ladeira, S. Massou, T. Parella, K. Miqueu, A. Amgoune, X. Ribas, D. Bourissou. ***Chemical Sciences***, 9, **2018**, 3932.

6- Organic Lewis Pairs Based on Phosphine and Electrophilic Silane for the Direct and Controlled Polymerization of Methyl Methacrylate: Experimental and Theoretical Investigations. W. N. Ottou, E. Conde-Mendizabal, A. Pascual, A-L. Wirotius D. Bourichon, J. Vignolle, F. Robert, Y. Landais, J-M. Sotiropoulos, K. Miqueu, D.Taton, ***Macromolecules***, 50 (3), **2017**, 762.