Laboratoire de Chimie
de Coordination du CNRS
www.lcc-toulouse.fr
205 route de Narbonne
BP 44099
31077 TOULOUSE CEDEX 4
France
T. +33 5 61 33 31 00
F. +33 5 61 55 30 03
UPR 8241

**Heterogeneous single atom catalysts for hydroformylation reaction**

Post-doctoral Research Fellow

Contact person: M. Rosa Axet rosa.axet@lcc-toulouse.fr

Start date: Before 1st March 2021

Are you interested in catalysis, have a PhD in chemistry and are you looking for an innovative, challenging research project? We are seeking a motivated researcher for a 12-month project funded by the CNRS (EMERGENCE@INC2021) on single atom catalysis. The research will be carried in the Engineering of metal nanoparticles group, possibly with international collaborators. For this project, we are looking for an independent and motivated candidate with a proven experience in either organometallic chemistry or material sciences and catalysis. Skills in anaerobic and anhydrous Schlenk techniques and in materials characterization techniques are an asset. We expect that the hired researcher will write the scientific articles and will be involved in the dissemination of results.

Hydroformylation (HF) reactions provide efficient pathways to form aldehydes from olefins by a reaction with syngas ($H_2$, CO). It is one of the most relevant industrial processes as aldehydes are important platform molecules for producing alcohols, amines, carboxylic acids, among others.[1] Rhodium and cobalt complexes, usually modified with phosphorus ligands, are commonly used as homogeneous catalysts for this reaction, due to their excellent performances in terms of activity and selectivity. Catalyst recycling of these homogeneous systems is well documented, and in fact applied at industrial scale, but are generally more complicated than the processes performed by typical heterogeneous catalyst. Several approaches have been explored to anchor well defined metal complexes on various supports but this has not been commercialized as yet.[1, 2] The synthesis of atomically dispersed single atoms is an emerging strategy to arrive at well defined metal centers on supports. Such approaches, allows to have isolated active sites and use precious metals efficiently in catalysis, combining thus the advantages of homogeneous and heterogeneous catalysis.[3] Very recently, rhodium based single-atom catalysts (SAC) have been reported active in HF.[4] Important open question, including the mechanism, the structure of the active species and how to control the selectivity of the reaction, have yet to be addressed. The aim of this project is to synthesise rhodium and cobalt SAC for HF applications, and answer these questions.

References: [1] Franke, R.; Selent, D.; Borner, A. Chem. Rev. 2012, 112 (11), 5675−732; van Leeuwen, Piet W. N. M., Claver, C. Rhodium Catalyzed Hydroformylation. [In: Catal. Met. Complexes, 2000; 22] , 2000, p.284 pp.-284 pp ; [2] Axet, M. R.; Castillon, S.; Claver, C.; Philippot, K.; Lecante, P.; Chaudret, B., Eur. J. Inorg. Chem. 2008, 3460-3466; [3] Ji, S.; Chen, Y.; Wang, X.; Zhang, Z.; Wang, D.; Li, Y., *Chem. Rev.* 2020, 10.1021/acs.chemrev.9b00818; Yang, X.-F.; Wang, A.; Qiao, B.; Li, J.; Liu, J.; Zhang, T. *Acc. Chem. Res.* 2013, *46*, 1740-1748; [4] Amsler, J.; Sarma, B. B.; Agostini, G.; Prieto, G.; Plessow, P. N.; Studt, F. *J. Am. Chem. Soc.* 2020, *142*, 5087-5096. Li, T.; Chen, F.; Lang, R.; Wang, H.; Su, Y.; Qiao, B.; Wang, A.; Zhang, T. *Angew. Chem., Int. Ed.* 2020, *59*, 7430-7434. Lang, R.; Li, T.; Matsumura, D.; Miao, S.; Ren, Y.; Cui, Y.-T.; Tan, Y.; Qiao, B.; Li, L.; Wang, A.; Wang, X.; Zhang, T. *Angew. Chem., Int. Ed.* 2016, *55*, 16054-16058. Wang, L.; Zhang, W.; Wang, S.; Gao, Z.; Luo, Z.; Wang, X.; Zeng, R.; Li, A.; Li, H.; Wang, M.; Zheng, X.; Zhu, J.; Zhang, W.; Ma, C.; Si, R.; Zeng, J. *Nat. Commun.* 2016, *7*, 14036.