



H2020-MSCA-ITN-2019-EJD www.ccimc.eu

PhD position available: 09/2020 - 08/2023

ESR3 Project: s-Block Metal-Mediated Hydroelementation

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Secondment host: **Italmatch Chemicals**, France

Context: The addition of H-E bonds of amines (hydroamination), phosphanes (hydrophosphanylation), and phosphane oxides (hydrophosphorylation) to multiple bonds (e.g. alkynes) represents an atom-economic reaction that requires a catalyst, usually a noble metal complex. The replacement of these catalysts with nonprecious metals is highly demanded. In the last years it has been proved that s-block metal complexes are able to promote these addition reactions regioselectively with a significantly increased reactivity for heterobimetallic catalysts (e.g. mixed K/Ca complexes). However, stereocontrol as well as steric and electronic control remain challenging tasks

Objectives: This project is aimed to achieve a substantial advance in the control and the practical applicability of such reactions by combining thorough computational exploration of their mechanism with experimental work.

The project relies on our complementary expertise in computational modelling of homogeneous catalysis at UAB,¹ and experimental s-block metal-mediated hydroelementations at FSU.²

Expected profile: We are looking for a highly motivated graduated student to work at the frontier of organic chemistry, coordination chemistry, homogeneous catalysis and computational modelling. Previous knowledge in organic synthesis as well as DFT calculations would be appreciated. Degree in Chemistry or Materials Science, and a Master in Chemistry will be mainly considered. A good level in English is required for daily and scientific communications. The applicant must not have resided or carried out his/her main activity (work, studies, etc.) in Spain for more than twelve months in the three years immediately prior to his/her recruitment. To be eligible for recruitment, the candidate must, at the date of recruitment, be within the first four years (full-time equivalent research experiences) of his/her research career and not to have a doctoral degree (see eligibility rules for applicants in www.ccimc.eu). **Applications will be considered up to 31st March 2020.**

This thesis will be part of an International Training Network (ITN) and more specifically a European Joint Doctorate (EJD), funded by the European Commission through the Marie Skłodowska-Curie Action (MSCA), entitled "Coordination Chemistry Inspires Molecular Catalysis" (CCIMC). This programme involves 15 joint theses. You are encouraged to consider all these thesis projects, to be consulted on the ITN-EJD website www.ccimc.eu.

Application: Please send a CV and a motivation letter together with two reference letters to agusti@klingon.uab.es, Gregori.Ujaque@uab.cat, m.we@uni-jena.de

[1] M. Westerhausen, B. E. Fener, P. Schüler, N. Ueberschaar, P. Bellstedt, H. Görls, S. Kriek. Scope and Limitation of the s-Block Metal-Mediated Pudovik Reaction. *Chem. Eur. J.* **2020**, doi.org/10.1002/chem.201905565.

[2] A. Couce-Rios, A. Lledós, I. Fernández, G. Ujaque. Origin of the Anti-Markovnikov Hydroamination of Alkenes Catalyzed by L-Au(I) Complexes: Coordination Mode Determines Regioselectivity. *ACS Catal.* **2019**, *9*, 848–858.

