



## Marie-Curie Ph.D. position for a double diploma from the University of York (UK) and the Université Toulouse 3 Paul Sabatier (France)

Title: "Polar substrates asymmetric hydrogenation and associated processes: role of the base"

**Project description**: In hydrogenation and transfer hydrogenation of polar substrates, new mechanistic views have recently emerged to account for the activity of system with non-

deprotonatable ligands, which nevertheless need a strong base for activity.<sup>1</sup> Through a combination of ligand synthesis, catalysis and mechanistic studies by advanced NMR, IR and DFT calculations, this project targets mechanistic understanding and the development predictive of tools for optimizing ligand the structure and maximising activity, enantioselectivity, stability and durability for specific prochiral substrates of industrial interest. The student will receive research training in organic chemistry (ligand synthesis), coordination chemistry, advanced spectroscopic techniques, computational approaches, mechanistic investigations, and homogeneous catalysis.



<sup>1</sup> (a) Dub, P. A.; Henson, N. J.; Martin, R. L.; Gordon, J. C. *J. Am. Chem. Soc.* **2014**, *136*, 3505. (b) Hayes, J. M.; Deydier, E.; Ujaque, G.; Lledós, A.; Malacea, R.; Manoury, E.; Vincendeau, S.; Poli, R. *ACS Catal.* **2015**, *5*, 4368.

Period of the fellowship: 1 October 2020 to 30 September 2023 (36 months).

**Funding**: The Horizon 2020 Marie Sklodowska-Curie Action (MSCA) Initial Training Network (ITN) programme of the European Commission funds this fellowship through the "European Joint Doctorate" (EJD) Network entitled "**Coordination Chemistry Inspires Molecular Catalysis**" (CCIMC), which offers a very competitive Ph.D. salary.

**Recruiting institution and training plan**: The Ph.D. student will be hired by and receive a salary from the University of York throughout the fellowship period, but will spend *ca.* half of the time at the Laboratoire de Chimie de Coordination (LCC), a research institution of CNRS associated to the Université de Toulouse, according to a bilateral agreement for the double diploma. In addition, two short secondment periods (3 months each) will take place with Prof. Agustí Lledós at the Universitat Autónoma Barcelona (Spain) to be trained on advanced computational approaches and with an industrial partner (Tecnalia, Spain) to work on the industrial applications of the developed catalysts. As part of the CCIMC ITN, the student will be exposed to a number of stimulating and rewarding network training events including tutorials, network workshops, international workshops and an international school.

**Eligibility**: The successful candidate must be in possession of a Master's degree, or complete one by the beginning of the Ph.D. thesis, and satisfy the MSCA mobility rule (no more than 12 months of work and/or residence in the recruiting institution Country within the last 3 years).

**Contacts**: Prof Simon Duckett (<u>simon.duckett@york.ac.uk</u>), Dr Jason Lynam (<u>jason.lynam@york.ac.uk</u>) and Dr John Slattery (<u>john.slattery@york.ac.uk</u>) at the University of York; Prof Rinaldo Poli (<u>rinaldo.poli@lcc-toulouse.fr</u>) at LCC-CNRS.



