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Position Description	
Reference	DC11
Title of the project	In situ and operando characterization of energetic aspects of Fe active sites in Enzyme-like MOF.
Recruiting Institution	University of Turin (Italy)
PhD jointly awarded by	University of Turin (Italy) and CNRS through University of Lille (France)
Additional secondment	Johnson Matthey (United Kingdom)
Expected Start Date (estimated)	01-02-2024
Job Offer Description	
Keywords	in situ and operando spectroscopies in controlled atmosphere and temperature, Bio-inspired catalysts, Metal Organic Frameworks, sMMO
Project Description	<p>DC11 will be hosted at University of Turin (Italy) and will be enrolled in the PhD school of the same institute, supervised by Prof. S. Bordiga. Part of the activity will be carried out during secondment periods, mainly at CNRS under the supervision of Prof. S. Paul to perform catalytic tests, as well as at JM (United Kingdom), to support Fe-MOFs (UiO-66/67) inside robust mesoporous scaffolds.</p> <p>The project will develop enzyme-mimicking MOFs stabilized in mesoporous scaffold to make robust, active and selective catalysts for light alkanes partial oxidation catalysts using N_2O, O_2, H_2O_2 as oxidants. Fe-MOF provided by DC11, will be supported in mesoporous scaffold in JM and screened in CNRS (Lille) to identify what are the most suitable substrates and reaction conditions. The most promising materials will be characterized in Turin combining a wide set of in situ and operando spectroscopies in order to address structure-properties relations. In collaboration with DC12, if suitable, a XAS campaign will be planned and made. Thanks to the results obtained a second generation of materials will be identified, made and tested.</p>
Objectives	<p>Science: Focus of the project will be to study with in situ approaches the enzyme-mimicking MOFs stabilized in mesoporous scaffold, to understand the effects of support-catalyst interaction and the nature of Fe species (oxidation state, aggregation, chemical and steric environments). To achieve this goal, in situ spectroscopies in controlled atmosphere and temperature, combined with volumetric measurements, will be developed. Moreover, operando measurements will be performed, to establish Fe site structure and catalytic performances correlations. All experiments will be carried out on composite materials made and tested by the candidate during the secondment periods.</p> <p>Training: Design of microporous materials: topological requirements and functionalization; Synthesis methods for porous materials and characterization via XRD, SEM/EDX, ATR, TGA); Hands-on training in catalyst pressing and sieving, reactor filling, testing and online detection using online mass flow controller, GC and MS; Physicochemical and engineering on solid-catalysts: catalytic cycles and heat/mass transfer Chemisorption techniques for the qualitative and quantitative assessment of surface metal species, Optical spectroscopies applied at catalysts: methods and applications;</p>



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	Chemisorption techniques for the qualitative and quantitative assessment of surface metal species; Synchrotron X-ray spectroscopy: principles, methods, applications to metal ions in porous networks; Additional technical and transferrable skills training network-wide.
Expected Results	1) synthesis, characterisation and testing of Fe-MOFs@mesoporous scaffold, combining characterization techniques (among which in situ/operando spectroscopy). 2) Disclose oxidation state, local geometry and coordination environment of Fe active sites aiming to select promising materials for the target reactions.
PhD Supervisors	Main supervisor: Prof. Silvia Bordiga (University of Turin, Italy) Co-supervisor: Prof. S. Paul (CNRS)
Vacancy requirements	
Qualifications	Eligible candidates must hold or be in the process of gaining a second level degree (Master's Degree level or equal qualification) which gives access to Ph.D. studies, including Chemistry, Physics, Materials Science, Chemical Engineering or a related discipline.
Requirements	The candidate must be eligible for enrolment in the PhD program at the date of the recruitment. Additional information on specific requirements and eligibility criteria of the PhD School of University of Turin can be found at the following link: https://www.phd.unito.it/do/home.pl/View?doc=Admission_Requirements.html
Languages	Successful candidates must have a high level of proficiency in written and spoken English, which will be assessed with the motivation letter and the interview, respectively.
Skills	The ideal candidate possesses: •synthetic skills •a strong background in physical chemistry, spectroscopy, catalysis; • propension to data analysis; • ability to adapt into multi-disciplinary work environments; • good team-working and communication skills.
Experience	Documented research experience in the field of heterogeneous catalysis will be considered as a plus at the selection stage.
Job Details	
Salary	Salary follows the rules in Marie Skłodowska-Curie Actions Work Programme. Gross salary per month: 3311.6 € € + 600 € mobility allowance
Other benefits	Other benefits: Gross family allowance: 495 € per month - if applicable* *The family allowance will also be made available to researchers whose parental status changes during their project.
Duration	36 months
Type of contract	Full time
Place of work	University of Turin (Italy, 20 months) CNRS (France, 12 months) Johnson Matthey (United Kingdom, 4 months)