

DC12 – Job Vacancy

Position Description	
Reference	DC12
Title of the project	Advanced electronic and structural characterization of bio-inspired Fe-based catalysts for light alkanes valorization via X-ray spectroscopy and theoretical modelling
Recruiting Institution	University of Turin (Italy)
PhD jointly awarded by	University of Turin (Italy) and University of Oslo (Norway)
Additional secondment	CNRS (France)
Expected Start Date (estimated)	01-02-2024
Job Offer Description	
Keywords	X-ray spectroscopy, Operando characterization, DFT modelling, Machine Learning, Bio-inspired catalysts, Metal Organic Frameworks, sMMO
Project Description	<p>DC12 will be hosted at University of Turin (Italy) and will be enrolled in the PhD school of the same institute, supervised by Prof. E. Borfecchia. Part of the activity will be carried out during secondment periods, mainly at University of Oslo (Norway) under the supervision of Res. Prof. D. Balcells to implement theoretical modelling tasks, as well as at CNRS (France), to learn how to properly handle bio-heterogeneous catalysts.</p> <p>The project aims at establishing and widely exploiting versatile characterisation protocols for the whole set of heterogeneous, biologic and hybrid catalysts developed in the DEMO network. The project will synergize experimental and theoretical tools, to identify structural motifs and electronic properties promoting activity/selectivity in light-alkane conversion over the DEMO bio-inspired Fe-catalysts. The main employed experimental techniques will include soft- and hard-X-ray absorption spectroscopy under in situ and operando conditions at synchrotron sources, while DFT modeling and machine learning approaches will guide and accelerate spectroscopic data interpretation.</p>
Objectives	<p>Science:</p> <ul style="list-style-type: none"> • Disclose oxidation state, local geometry and coordination of Fe sites in Fe-MOF catalysts at key pretreatment/reactivity steps, via theory-assisted X-ray spectroscopy studies using both hard and soft X-rays. • Quantitatively analyze the large datasets from synchrotron measurement by DFT-assisted simulations and emerging statistical/machine-learning-based approaches. • Extend the developed protocols to hybrid systems, with an emphasis on biologic catalysts and related challenges (Fe dilution, radiation damaging). <p>Training:</p> <ul style="list-style-type: none"> • Design, plan and perform X-ray spectroscopy at synchrotron. • Comprehend Fe electronic/structural properties under reaction and optimised in terms of sample properties. • Pretreat and analyse XANES, EXAFS, XES, NEXAFS data with dedicated codes / customised routines. • Build up reliable models of active sites and reaction intermediates, and exploitation to simulate or fit spectroscopic data. Additional technical and transferrable skills training network-wide.
Expected Results	<ul style="list-style-type: none"> • Achieve detailed understanding of the local geometric/electronic structure and reactivity of active Fe-sites in selected enzyme-mimicking MOFs, to assess synthesis effectiveness into targeted first coordination sphere environment/nuclearity and structure-activity relationships. • Establish protocols for X-ray spectroscopy on bio-heterogeneous



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	catalysts, primarily targeting impact of enzyme immobilisation on Fe local properties in most promising systems.
PhD Supervisors	Prof. Elisa Borfecchia (University of Turin, Italy) Res. Prof. David Balcells (University of Oslo, Norway)
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	<p>The candidate must be eligible for enrolment in the PhD program at the date of the recruitment.</p> <p>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</p> <p>Export control: "The position's subject area may require licensing under the Norwegian Export Control Act. In order to be considered for the position, it is a prerequisite that UiO must be able to be granted such licence. https://www.uio.no/english/studies/admission/master/export-control.html"</p> <p>Grade requirements: "The grade requirements of the position are as follows: the average grade point for courses included in the Bachelor's degree must be equivalent to C or better in the Norwegian educational system the average grade point for courses included in the Master's degree must be equivalent to B or better in the Norwegian educational system; the Master's thesis must have the equivalent to grade B or better in the Norwegian educational system."</p> <p>English skills: Demonstrated fluency in English. Details of English-language requirements for applicants from non-EU/EEA countries and exemptions from the requirements can be found here: https://www.mn.uio.no/english/research/phd/regulations/regulations.html#toc8"</p>
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	<p>The ideal candidate possesses:</p> <ul style="list-style-type: none"> • a strong background in physical chemistry, spectroscopy, quantum chemistry; • propension to data analysis/modelling tasks; • ability to adapt into multi-disciplinary work environments; • good team-working and communication skills. <p>Knowledge of a modern programming language (e.g., Python) and machine learning techniques is also an asset.</p>
Experience	Documented research experience in the field of X-ray spectroscopy and/or computational modelling, with an emphasis on their applications in catalysis, will be considered as a plus at the selection stage.
Job Details	
Salary	<p>Salary follows the rules in Marie Skłodowska-Curie Actions Work Programme.</p> <p>Gross salary per month: 3311.6 € € + 600 € mobility allowance</p>
Other benefits	<p>Other benefits: Gross family allowance: 495 € per month - if applicable*</p> <p>*The family allowance will also be made available to researchers whose parental status changes during their project.</p>



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Duration	36 months
Type of contract	Full time
Place of work	University of Turin (Italy, 20 months) University of Oslo (Norway, 12 months) CNRS (France, 4 months)