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DC8 – Job Vacancy

Position Description	
Reference	DC8
Title of the project	High-throughput screening of enzyme-mimicking MOFs and their optimization towards alcohols production
Recruiting Institution	CNRS (Lille, France)
PhD jointly awarded by	University of Lille (France) and University of Oslo (Norway)
Additional secondment	University of Basque Country (Spain)
Expected Start Date (estimated)	01-11-2023
Job Offer Description	
Keywords	High-throughput screening; Metal-organic frameworks (MOFs); Heterogeneous catalysts; Alkane oxidation
Project Description	The Doctoral Candidate will be hosted mainly at the Unit of Catalysis and Solid-state Chemistry (UCCS, Lille, France) and will be enrolled in the PhD school of the University of Lille, supervised by Dr. Fabio BELLOT NORONHA. Part of the work will be carried out at University of Oslo during secondment periods, under the supervision of Prof. D. Balcells and at University of Basque Country under supervision of Prof. I. Aguirrezabal. The project aims at investigating the performance of MOFs containing mono-Fe or di-Fe complex sites and methane monooxygenases (sMMO) immobilized on MOFs for the oxidation of short-chain alkanes (C_1-C_4) to alcohols. High-throughput catalytic testing under different reaction conditions will be carried out to establish a correlation between physicochemical and biological properties and catalyst activity, selectivity and stability, supported by a ML approach gained though theoretical calculations. Most promising catalysts will be tested under capillary reaction conditions.
Objectives	**Science:** • Synthesis of MOFs containing i) mono-Fe or ii) di-Fe complex sites; • Theoretical studies describing the oxidation of light alkanes to alcohols by Fe complexes confined into MOF nanopores • The UiO-66/67 Zr-based MOF catalysts and sMMO derivatives will be tested for C_1-C_4 alkane selective oxidation to alcohols in a high-throughput (HTE) equipment. Large ranges of substrates and reaction conditions (T, P or flow) will be evaluated; • catalyst characterization (before and after tests) and conversion and selectivity data under solvation at EHU. **Training:** MOF synthesis and characterization • Enzyme chemistry. • Theoretical and practical aspects for high-throughput screening. • Reactor Engineering. • Catalysis of C1 Chemistry. • Data for ML. • Fundamentals on catalyst characterization.
Expected Results	• The best catalysts and the best sets of operating conditions, in terms of catalyst features or reaction phases, to reach the highest yields in alcohols from different light alkanes substrates will be identified; • Determination of structure-activity correlations from HTE experiments; • New methods of treatment of data issued from HTE, implying ML and AI approaches will be developed.
PhD Supervisors	Dr. Fabio BELLOT NORONHA (Centrale Lille - CNRS, France) Prof. D. BALCELLS (University of Oslo, Norway)

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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 Material Sciences, Biochemistry, Chemical Engineering, Material Sciences 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 Lille can be found at the following link: https://edsmre.univ-lille.fr/rejoindre-led/candidature **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" **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." **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"
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: • a strong background in material sciences, and catalysis; • ability to adapt into multi-disciplinary work environments; • good team-working and communication skills.
Experience	Experience in the manipulation of catalytic tests, and in the analysis of mixtures of organic molecules by chromatography.
Job Details	
Salary	Salary follows the rules in Marie Skłodowska-Curie Actions Work Programme. Gross salary per month: 3957.6 € + 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	CNRS (Lille, France, 21 months) UIO (Norway, 12 months) UPV/EHU (Spain, 3 months)

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