

## DC2 – Job Vacancy

Position Description	
<b>Reference</b>	DC2
<b>Title of the project</b>	Kinetic and mechanistic studies on enzyme-mimicking MOFs with mono-Fe or di-Fe sites.
<b>Recruiting Institution</b>	University of Oslo (Norway)
<b>PhD jointly awarded by</b>	University of the Basque Country (Spain)
<b>Additional secondment</b>	University of Turin (Italy)
<b>Expected Start Date (estimated)</b>	01-02-2024
Job Offer Description	
<b>Keywords</b>	Catalytic testing, reaction mechanisms, transient kinetics, isotopic labelling, titration, site-function correlations
<b>Project Description</b>	Catalytic testing is the ultimate characterization tool for the enzyme-mimicking, MOF-based Fe catalysts developed in DEMO. Focus will be set on transient methods aimed at elucidating reaction rates, reaction schemes and mechanisms of partial oxidation reactions of light alkanes and alcohols over catalysts containing mono- and di-Fe sites. Titration of specific sites will be applied to unravel the role played by Fe sites and by functional groups in the 1 <sup>st</sup> and 2 <sup>nd</sup> coordination sphere of the Fe sites. Operando spectroscopy will be applied to identify reaction intermediates and to elucidate changes in oxidation states and coordination environment under reactive conditions.
<b>Objectives</b>	<p><b>Science:</b></p> <ol style="list-style-type: none"> <li>1) Establish site-performance correlations to activate O<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>O, and in-situ produced H<sub>2</sub>O<sub>2</sub> with light alkanes (targeting CH<sub>4</sub>) in MOFs from DC1.</li> <li>2) Determine the number and turnover rate of active sites on the catalyst surface, to convert alkanes as well as their primary oxidation product, alcohols, to products.</li> <li>3) Operando spectroscopy will be combined with transient methods to identify intermediates and rate-limiting steps.</li> <li>4) Comparison of the kinetics and mechanism of light alkane activation over kinetic and mechanistic studies in enzyme-mimicking MOFs embedded on aluminosilicate carriers (at EHU), enhancing the understanding of inter-site influence in enzyme catalysis.</li> </ol> <p><b>Training:</b></p> <ol style="list-style-type: none"> <li>1) Transient studies under flow (steady-state Isotopic Transient Kinetic Analysis (SSITKA) and near-vacuum (TAP) conditions applied to oxidation reactions (UiO),</li> <li>2) Integration of titration mechanistic analyses in transient methods (EHU)</li> <li>3) Operando spectroscopic techniques (TUR).</li> </ol> <p>Additional technical and TS training network-wide.</p>



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<b>Expected Results</b>	<p>1) Detailed kinetic and mechanistic insight in light alkane and alcohol oxidation over MOFs containing mono-Fe and di-Fe sites where Fe is coordinated to 2 or 4 N-binding ligands.</p> <p>2) Verification/falsification of optimal Fe sites (mono-/di-Fe) and coordination spheres in 2nd generation Fe-MOFs, predicted by ML</p>
<b>PhD Supervisors</b>	<p>Main supervisor: Prof. Unni Olsbye (University of Oslo, Norway)</p> <p>Co-supervisor: Prof. Iker Agirrezabal-Telleria (University of the Basque Country, Spain)</p>
<b>Vacancy requirements</b>	
<b>Qualifications</b>	Completed BSc and MSc degrees (equivalent to 4 years of study if given by an institution outside Norway). The BSc or the MSc should be in one of these fields: chemistry, materials science, or nanotechnology.
<b>Requirements</b>	<p>Previous experience with catalytic testing, preferably reactions at gas-solid interfaces.</p> <p>Training in one or more of the following areas will be a plus: Organic chemistry, use of gas chromatography, mass spectrometry, spectroscopic techniques (IR, UV-VIS).</p> <p>The average BSc grades should be equivalent to or higher than C in the Norwegian education system, and the average MSc grades should be equivalent to or higher than B in the Norwegian education system.</p> <p>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. <a href="https://www.uio.no/english/studies/admission/master/export-control.html">https://www.uio.no/english/studies/admission/master/export-control.html</a></p>
<b>Languages</b>	<p>Fluent in English at all levels (read, write, and speak)</p> <p>Details of English-language requirements for applicants from non-EU/EEA countries and exemptions from them can be found here: <a href="https://www.mn.uio.no/english/research/phd/regulations/regulations.html#toc8">https://www.mn.uio.no/english/research/phd/regulations/regulations.html#toc8</a></p>
<b>Skills</b>	<p>Excellent communication abilities through both manuscripts and presentations (text and visual contents)</p> <p>Capacity to work independently</p> <p>Ability to work in teams</p> <p>Curiosity-driven, creative thinking</p> <p>Discussing in interdisciplinary environments</p> <p>Giving feedback based on constructive criticism</p>
<b>Job Details</b>	
<b>Salary</b>	<p>Salary follows the rules in Marie Skłodowska-Curie Actions Work Program</p> <p>Salary NOK 532 200 – 575 400 per annum, depending on qualifications in a position as PhD Research fellow (position code 1017).</p>
<b>Other benefits</b>	<p>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>
<b>Duration</b>	36 months



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<b>Type of contract</b>	Full time
<b>Place of work</b>	University of Oslo (Norway, 24 months) University of the Basque Country (Spain, 9 months) University of Turin (Italy, 3 months)