

### DC5 – Job Vacancy

Position Description	
Reference	DC5
Title of the project	Integrated catalyst-reactor-process engineering for alkane oxidation under solvation phenomena.
Recruiting Institution	National Institute of Chemistry (Ljubljana)
PhD jointly awarded by	National Institute of Chemistry through the University of Ljubljana (Slovenia) and University of Basque Country (Spain)
Additional secondment	Johnson Matthey (United Kingdom)
Expected Start Date (estimated)	01-02-2024
Job Offer Description	
Keywords	In-silico production of materials, DFT modelling and screening, computational fluid dynamics (CFD), multi-scale modelling
Project Description	<p>DEMO will integrate Machine Learning (ML), organic chemistry, modelling, high-throughput engineering and in-situ spectroscopy to discover enzyme-mimicking Metal-Organic Frameworks (MOFs):</p> <ul style="list-style-type: none"> <li>• Virtual High-Throughput Screening (VHTS) to generate a dataset with active species: ML, enzyme sequencing and MOF design to learn the fundamental requirements for alkane, specifically methane, activation into alcohols.</li> <li>• Test the dataset value: screen large and diverse samples via experimental high-throughput engineering and modelling.</li> <li>• Understand testing outputs: combine advanced in-situ and operando spectroscopy, poisoning kinetics and modelling to elucidate the role and to improve each active component both during synthesis and catalysis.</li> <li>• Optimise synthetic materials towards biological analogues: explore new capillary solvation using gas-molecules.</li> </ul>
Objectives	<p><b>Science:</b></p> <ol style="list-style-type: none"> <li>1) In-silico production of materials with MOFs from DC1-3.</li> <li>2) DFT modelling and screening for CH<sub>4</sub> activation by high throughput computation with promising alkane oxidation activity/selectivity/stability.</li> <li>3) Computational fluid dynamics (CFD), providing the gaseous flow and heat/mass transfer features.</li> <li>4) Data for catalyst synthesis via three iterations with DC4.</li> <li>5) Optimal clustering by DFT, KMC and MKM models (surface reaction dynamics).</li> <li>6) Multi-scale modelling approaches and reactor/process to reflect capillary solvation.</li> </ol> <p><b>Training:</b></p> <p>development of high throughput computation models adapted to include mass transfer phenomena in capillaries. Simulation of reactor fluid-dynamics, combining experimental inputs into models. Bringing characterisation data into models to have a complete overview of both kinetic and transport effects. Additional technical and TS training network-wide.</p>



DEMO

Funded by  
the European Union

<b>Expected Results</b>	DC5 project (Integrated catalyst-reactor-process engineering for alkane oxidation under solvation phenomena) expected results: 1) In silico preparation of XY/Z (X = function 1; Y = ligand/complex 2; Z = MOF type) with diverse size, morphology and distribution. 2) High single pass reactor conversion for CH <sub>4</sub> -to-CH <sub>3</sub> OH vs. plant scale. 3) Dynamic process operation with integrative optimisation for catalyst materials; specifically multi-scale-wise. 4) A new established workflow to be translated to DC4.
<b>PhD Supervisors</b>	Supervisor: Dr. Matej Huš (National Institute of Chemistry) Co-supervisor: Prof. Dr. Pedro Luis Arias (University of Basque Country) Stephen Poulston (Johnson Matthey)
<b>Vacancy requirements</b>	
<b>Qualifications</b>	BSc and MSc degrees (equivalent to 4 years of study). The BSc or the MSc should be in one of these fields: chemical engineering, chemistry, materials science, or nanotechnology, or any related fields.
<b>Requirements</b>	Previous experience with chemical reaction engineering, catalytic material design or characterization at gas-solid interfaces.
<b>Languages</b>	Fluent in English at all levels (read, write, and speak)
<b>Skills</b>	Excellent communication abilities through both manuscripts and presentations (text and visual contents) Capacity to work independently Ability to work in teams Curiosity-driven, creative thinking Discussing in interdisciplinary environments Giving feedback based on constructive criticism
<b>Job Details</b>	
<b>Salary</b>	Salary follows the rules in Marie Skłodowska-Curie Actions Work Programme.  Gross salary per month 2832.2 € + 600 € mobility allowance + 495 € family allowance
<b>Other benefits</b>	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.
<b>Duration</b>	36 months
<b>Type of contract</b>	Full time
<b>Place of work</b>	National Institute of Chemistry (Slovenia, 23 months) University of Basque Country (Spain, 9 months) Johnson Matthey (United Kingdom, 4 months)