DEMO

Funded by the European Union

DC4 – Job Vacancy

Position Description	
Reference	DC4
Title of the project	*Ab initio* Atomistic Micro-kinetic Modelling of Direct Stepwise Conversion of Methane.
Recruiting Institution	National Institute of Chemistry (Ljubljana)
PhD jointly awarded by	National Institute of Chemistry through the University of Ljubljana (Slovenia) and University of Turin (Italy)
Additional secondment	University of Oslo (Norway)
Expected Start Date (estimated)	01-01-2024
Job Offer Description	
Keywords	Kinetic Monte Carlo, ab initio micro-kinetic modelling, transient kinetics, reactor configurations and characterisations, technical and TS training network-wide
Project Description	DEMO will integrate Machine Learning (ML), organic chemistry, modelling, high-throughput engineering and in-situ spectroscopy to discover enzyme-mimicking Metal-Organic Frameworks (MOFs): • 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. • Test the dataset value: screen large and diverse samples via experimental high-throughput engineering and modelling. • 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. • Optimise synthetic materials towards biological analogues: explore new capillary solvation using gas-molecules.
Objectives	**Science**: 1) Elucidate active-sites for alkanes-to-alcohol (from C2-C4 alkanes into CH4), via kinetic Monte Carlo, ab initio micro-kinetic modelling and transient kinetics, reactor configurations and characterisations. 2) Prepare in-silico model Fe-catalysts for diverse alkane activation routes. Selectivity prioritised via metal–support tuning to suppress over-oxidation. 3) CH4 catalysis and CH3OH desorption on MOFs at different pressures. Idealised micro-kinetics to screen catalysts and process conditions. 4) Translate structural findings to DC 1-3 and 8-10. **Training:** Monte Carlo, ab initio chemical micro-kinetic modelling to develop kinetic models adapting to outputs from DC2, DC9, DC11. Simulating theory-driven X-ray spectroscopy data to optimise catalyst preparation and ab initio models. Additional technical and TS training network-wide.
Expected Results	DC4 project (Ab initio Atomistic Micro-kinetic Modelling of Direct Stepwise Conversion of Methane) expected results: 1) Prepare metal/support models via atom-scaling (40–100 atoms). 2) Determination of catalytically active sites. 3) Model-based catalysts tested for direct methane to methanol. The ab

	initio-based micro-kinetic model of chemical looping, with active site formation, CH4 reaction and CH3OH desorption. 4) Correlation between the catalyst preparation, CH3OH yields and site nature via spectroscopy.
PhD Supervisors	Supervisor: Prof. Dr. Blaž Likozar (National Institute of Chemistry) Co-supervisor: Assoc. Prof. Elisa Borfecchia (University of Turin) Prof. David Balcells (University of Oslo)
Vacancy requirements	
Qualifications	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.
Requirements	Previous experience with chemical reaction engineering, catalytic material design or characterization at gas-solid interfaces.
Languages	Fluent in English at all levels (read, write, and speak)
Skills	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
Job Details	
Salary	Salary follows the rules in Marie Skłodowska-Curie Actions Work Programme. Gross salary per month 2832.2 € + 600 € mobility allowance + 495 € family 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	National Institute of Chemistry (Slovenia, 18 months) University of Turin (Italy, 12 months) University of Oslo (Norway, 6 months)