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Position Description	
Reference	DC10
Title of the project	Optimization of catalytic performance for alkane to alcohol production via capillary liquid nanoshell formation
Recruiting Institution	University of Basque Country (Bilbao, Spain)
PhD jointly awarded by	University of Basque Country (Spain) and National Institute of Chemistry via University of Ljubljana (Slovenia)
Additional secondment	ProfMOF (Norway)
Expected Start Date (estimated)	01-02-2024
Job Offer Description	
Keywords	Catalytic testing, solid-catalysis, capillary liquid formation, site-function correlation, DFT
Project Description	This project will evaluate how capillary nanoshells, formed via condensation from C ₂ -C ₄ alkanes or CH ₃ OH from CH ₄ , affect catalyst reactivity and stability. We will determine the conditions (P, T, type of molecule/mixtures) to achieve pore condensation in 1-6 nm pores (structured SiAl capillaries or MOFs). We will evaluate how the transition gas into a mixed gas-liquid or capillary liquids affects the reactivity (via kinetically-relevant TS solvation) or the stability (by suppressing the formation of deactivating species or protecting active species). The experimental results will also be modelled to understand the catalytic consequences of capillary liquids, helping optimize the performance for the production of alcohols.
Objectives	<p>Science:</p> <p>This project will tackle the formation of capillary liquids using different approaches:</p> <ul style="list-style-type: none"> - The characterization of porous materials and their correlation to the formation of capillary liquids - Effect of pore environment, pore-filling and reaction conditions on catalytic performance - Establish site-function and capillary liquid correlations via coupled to advanced theoretical modelling - Study of the feasibility of developed materials and reaction conditions at industrially relevant conditions <p>Training:</p> <p>Synthesis and characterisation training on techniques to determine pore-condensation phenomena such as the adsorption of common molecules (N₂, Ar) but also more complex systems involving H₂O, H₂O₂, CH₄ via physisorption techniques, high-pressure TGA or indirect measures such as tomography. Secondments will permit translating experimental evidences to modelling conditions. Additional technical and TS training network-wide.</p>



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Expected Results	1) capillary condensation in UIO/PMOF and MIT's samples are expected to show analogous liquid-effects as for enzymes, enhancing catalytic turnover compared to gas-conditions and reducing overoxidation of products. 2) These effects will turn more stable catalysts, evaluated under industrially-relevant conditions. 3) Mechanistic effects will be modelled to understand solvation in solids.
PhD Supervisors	Prof. Miryam Gil-Calvo (University of Basque Country, Bilbao, Spain) Prof. Blaž Likozar (National Institute of Chemistry, Ljubljana, Slovenia)
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: 3104.2 € + 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	- Department of Chemical and Environmental Engineering, University of Basque Country, Bilbao, (Spain, 20 months) - National Institute of Chemistry (Slovenia, 12 months)) - ProfMOF (Norway, 4 months)