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DC9 – Job Vacancy

Position Description	
Reference	DC9
Title of the project	Determination of the role of catalytic sites in MOFs via selective titration and spectroscopy
Recruiting Institution	University of Basque Country (Bilbao, Spain)
PhD jointly awarded by	University of Basque Country (Spain) and University of Turin (Italy)
Additional secondment	Johnson Matthey (United Kingdom)
Expected Start Date (estimated)	01-01-2024
Job Offer Description	
Keywords	Catalytic testing, solid-catalysis, mechanistic analyses, titration, site-function correlation, in-situ spectroscopy
Project Description	This project will elucidate the role of active moieties in Fe-based MOFs or enzyme-mimicking Zn-MFU-4l designed in collaboration with M. Dinca at MIT (USA) for CH_4 activation. It will bring MOF ingredients (ligands, metals) to grow MOFs inside SiAl mesopores (MCM-41) and yield robust catalysts at Johnson Matthey. Transient experiments will determine oxidant (O_2, H_2O_2, H_2O) effects during titration. In addition, in-situ titration experiments, fed under controlled conditions will qualitatively evaluate transitions in CH_4 conversion or CH_3OH selectivity. Such assessments will be helped by in-situ spectroscopy experiments under relevant catalytic conditions.
Objectives	**Science:** This project will tackle the elucidation of active-site role via different perspectives, with the following specific objectives: - Determine the individual and synergetic role of active-sites. - Assess the evaluation of active species and their possible deactivation - Establish site-function correlations via kinetic and spectroscopic evidence - Bring studied MOF catalysts into industrially relevant supports **Training:** Experimental design and catalytic activity measurement through transient kinetics and equipment for testing (microactivity, GC-MS, pressurized units) or characterisation (IR, TGA, NRM or chemisorption). Secondments will train key aspects related to in-situ spectroscopy, enhancing obtained catalytic data. In addition, DC will receive relevant transferable skill training in scientific communication, ethics in research, grant writing or through secondment periods. Additional technical and TS training network-wide.
Expected Results	1) titration experiments will clarify the isolated or synergetic role of active species on the surface. 2) The binding strength, for each molecule, will also determine the nature of each active site. 3) Combining in-situ spectroscopic data with modelling data will yield a thorough understanding of enzymatic or MOF functions in catalysis. 4) Outputs will serve to improve DC1-3 synthesis methods.
PhD Supervisors	Prof. Iker Aguirrezabal-Telleria (University of Basque Country, Bilbao, Spain) Prof. Silvia Bordiga (University of Turin, Italy)

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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) - University of Turin, Italy (12 months) - Johnson Matthey, United Kingdom (4 months)