DEMO PROJECT - ***Project Week #3 (Bilbao, Spain)***

Day 1. Wednesday, October 7th, 2026

9:00 – 9:15 Visitors reception

9:15 – 10:00 Solvation and confinement effects in microporous materials: characterization and testing purposes - Iker Aguirrezabal (University of Basque Country, Spain)
10:00 – 10:30 Determination of the role of catalytic sites in MOFs via selective titration and spectroscopy - Leonardo Spuri (University of Basque Country, Spain)
10:30 – 11:00 Optimization of catalytic performance for alkane to alcohol production via capillary liquid nanoshell formation - Morena Chiariotti (University of Basque Country, Spain)

11:00 – 11:30 Coffee break

11:30 – 12:15 The Cost of Catalysis: What it means and how to bring it down through Innovation - Sean McCarthey, Beatriz Dominguez (Johnson Matthey, United Kingdom)
12:15 – 12:45 Tailored immobilization of oxidation enzymes onto MOF to synthetize stable bio-heterogeneous catalysts for light-chain alkane oxidation - Jana Vojčíková (Centre National de la Recherche Scientifique, France)
12:45 – 13:15 Screening, engineering and development of peroxygenases as catalysts for alkane oxidation to alcohols - Myint Toe (Johnson Matthey, United Kingdom)

13:15 – 14:45 Lunch break

14:45 – 15:15 Synthesis of sMMO-inspired MOFs for C-H activation - Malik Vincent (University of Oslo, Norway)
15:15 – 15:45 In situ and operando characterization of energetic aspects of Fe active site in enzyme-like MOF - Bezayet Tesfaye (University of Turin, Italy)

Free evening

Day 2. Thursday, October 8th, 2026

8:30 – 9:15 Modelling of Catalytic Reactors for Integration into Process Engineering via Aspen Plus – Miryam Gil (University of Basque Country, Spain)
9:15 – 9:45 Integrated catalyst-reactor-process engineering for alkane oxidation under solvation phenomena - Bahador Kazemi (National Institute of Chemistry, Slovenia)
9:45 – 10:15 High-throughput screening of enzyme-mimicking MOFs and their optimization towards alcohol production – Lucas Bitencourt Theodoroviez (Centre National de la Recherche Scientifique, France)
10:15 – 10:45 Fe-based bio-inspired catalysts characterization via X-ray spectroscopy and theoretical modelling - Flavie Le Rai (University of Turin, Italy)

10:45 – 11:15 Coffee break

11:15 – 12:00 Predictive and Generative AI for the Transition Metals - David Balcells (University of Oslo, Norway)
12:00 – 12:30 Computational Engineering of Iron Metalated MOFs for the Catalytic Oxidation of Light Alkanes - Michael Augello (University of Oslo, Norway)
12:30 – 13:00 Atomistic and microkinetic modelling of the activation of methane, ethane and propane on heterogeneous iron-organic framework catalysts - Yasmeen Iqbal (National Institute of Chemistry, Slovenia)

13:00 – 14:30 Lunch break

14:30 – 15:00 Fe- and Cu- supported on carbon catalysts prepared from the pyrolysis of MOFs - Diya Mandal (Centre National de la Recherche Scientifique, France)
15:00 – 15:30 Project management
15:30 – 16:30 What lies at the heart of grant writing - Lotte Jaspers (Yellow Research, the Netherlands)

Project dinner

Day 3. Friday, October 9th, 2026

Appointment at the School of Engineering of Bilbao (San Mames Stadium) at 9:00 for the departure to Urdaibai

11:00 – 12:30 First activity

Maritime route by Kayak. If the weather is not good, access to an adventure park

14:00 – 15:30 Lunch break

15:30 – 17:30 Second activity

Hike in Gaztelugatxe

Departure to Bilbao

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