DEMO

Funded by the European Union

DC3 – Job Vacancy

Position Description	
Reference	DC3
Title of the project	Computational Engineering of Iron Metalated MOFs for the Catalytic Oxidation of Light Alkane
Recruiting Institution	University of Oslo (Norway)
PhD jointly awarded by	University of Oslo (Norway) and University of Ljubljana (Slovenia)
Additional secondment	Open
Expected Start Date (estimated)	01-02-2024
Job Offer Description	
Keywords	DFT, molecular engineering, MOF, machine learning, multiscale modeling, high-throughput virtual screening
Project Description	DFT methods will be used to study and engineer the nanopores within MOFs with the aim of mimicking the catalytic properties of enzyme oxidizing light alkanes. A special focus will be put on the UiO Zr MOFs metalated with iron for the oxidation of methane. Both SBU and linker metalation will be considered, together with the functionalization of proximal moieties playing a co-catalytic role. The associated chemical spaces will be explored through the generation of large datasets, which will be leveraged with machine learning methods. Multiscale modeling will be used to relate the macroscopic properties of these materials with their microscopic structure at the atomic level.
Objectives	**Science:** 1) Understand the relationship between metalation and catalytic activity 2) Identify co-catalytic moieties boosting the reactivity of the metal sites 3) Map the chemical space of metallated MOFs 4) Model the associated catalytic processes over multiple scales **Training:** 5) DFT modeling of reaction pathways 6) Use of cluster and periodic models 7) MD simulations for conformational space exploration 8) Statistical data analysis 9) Representations and models for machine learning 10) HPC, including automation protocols
Expected Results	1) Structure-activity/selectivity/robustness relationships 2) Reaction mechanisms including confinement and co-catalysis 3) Metalated MOF datasets including quantum properties 4) Multiscale kinetic models
PhD Supervisors	Main supervisor: Res. Prof. David Balcells (University of Oslo, Norway) Co-supervisor: Prof. Blaz Likozar (National Institute of Chemistry, Slovenia)
Vacancy requirements	
Qualifications	Completed BSc and MSc degrees (equivalent to 4 years of study if given by an institution outside Norway). The BSc or the MSc should be in one of these fields: chemistry, materials science, or nanotechnology.

Requirements	Previous experience with computational chemistry. Training in one or more of the following areas will be a plus: DFT modeling with both cluster and periodic models, DFT modeling of open-shell systems, software engineering, data science, machine learning, use of HPC facilities. The average BSc grades should be equivalent to or higher than C in the Norwegian education system, and the average MSc grades should be equivalent to or higher than B in the Norwegian education system. The position's subject area may require licensing under the Norwegian Export Control Act. In order to be considered for the position, it is a prerequisite that UiO must be able to be granted such licence. https://www.uio.no/english/studies/admission/master/export-control.html
Languages	Fluent in English at all levels (read, write, and speak) Details of English-language requirements for applicants from non-EU/EEA countries and exemptions from them can be found here: https://www.mn.uio.no/english/research/phd/regulations/regulations.html#toc8
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
Experience	Computational modeling of molecules and/or surfaces and/or bulk materials, preferably in an HPC environment and with a focus on reactivity
Job Details	
Salary	Salary follows the rules in Marie Skłodowska-Curie Actions Work Program Salary NOK 532 200 – 575 400 per annum, depending on qualifications in a position as PhD Research fellow (position code 1017).
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	University of Oslo (Norway, 24 months) National Institute of Chemistry (Slovenia, 9 months) Additional secondment (3 months)