MS01: **Energy and Environmental Materials: Simulation and Machine Learning**

Organizers: Marie-Christine Record (IM2NP), Pascal Boulet (IM2NP)

Invited Speakers: Dr. Peter Wiecha (LAAS, Toulouse), Dr. Celine Barreteau (ICMPE, Thiais), Dr. Luca Messina (CEA, Cadarache)

The development of innovative materials for energy and environmental applications is a major challenge in the context of the energy transition and sustainable development. To overcome the limitations of traditional trial-and-error approaches, the combination of numerical simulations (DFT, molecular dynamics, multiscale methods) and machine learning techniques now offers promising perspectives for accelerating materials discovery, high-throughput screening, and inverse materials design.

This mini-symposium will bring together contributions focused on the modeling, property prediction, and optimization of materials for energy and environmental applications, with an emphasis on simulation and modeling approaches, with or without experimental support. Interdisciplinary approaches at the interface of condensed matter physics, chemistry, materials science, and data science will be particularly encouraged. Topics will include, but are not limited to, computational screening, machine learning applied to materials, and the study of energy conversion and storage mechanisms as well as pollution mitigation processes, based on computational approaches alone or in combination with experimental data.