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S E M I N A I R E

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"Self-Assembly and Phase Transitions of Metal-Organic Framework from a Modelling Standpoint"

The unique structural diversity of metal-organic frameworks (MOFs) makes them very promising for applications in many environmental and industrial fields, such as carbon capture, drug delivery and generation of renewable energies. In this seminar, I will discuss recent works in my group focused on better understanding the physico-chemical basis underlying the MOF synthesis process. This is a challenging task, as the MOF synthesis landscape is very complex: starting from a given ligand and metal, MOFs with different topologies, defects, morphologies can be obtained. All these properties are relevant because they affect the mass transport, catalytic activity or stability of the material, to cite a few examples. We have studied the synthesis process and phase transitions of zeolitic-imidazolate frameworks via the implementation of multi-scale modelling and metadynamics techniques combined with data-driven analyses.[1-4] This enabled us to unveil mechanistic details of these reactive processes at the molecular level as well as to contribute to determining the complex phase diagram of these materials.

[1] S. R. G. Balestra and R. Semino; The Journal of Chemical Physics, 157, 184502 (2022)
[2] E. Méndez and R. Semino; Journal of Materials Chemistry A, 12, 4572 - 4582 (2024)
[3] E. Méndez and R. Semino; Journal of Materials Chemistry A, 12, 31108-31115 (2024)
[4] E. Méndez and R. Semino; arXiv:2411.04884

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14h00

Salle des conférences