Modelling the Self-Assembly of Metal-Organic Frameworks

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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 lecture, 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.[1] 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 (ZIFs), a family of MOFs formed by Zn^{2+} and imidazolate-based ligands, via the implementation of multiscale modelling and metadynamics techniques combined with data-driven analyses.[2-6] This enabled us to unveil mechanistic details of these reactive processes at the molecular level[2,3,5-7] as well as to contribute to determining the complex phase diagram of these materials.[4] The lecture will focus on our progress concerning understanding the molecular mechanism of self-assembly of Zn^{2+} and imidazolate ions to form ZIFs, going from the formation simple metal ion/ligand complexes,[2,5,6] to nucleation,[2,6] and growth.[5,7]

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