Supramolecular metallo-organic cages: a rational journey to new efficient catalysts

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Selective catalysis in supramolecular confined spaces has emerged as an innovative approach capable of responding to the urgent need for catalysts with excellent efficiency as well as high selectivity and conversion. The nanoconfined environment allows to modulate the chemical-physical properties in a fine and controlled way, to increase reaction rates and selectivity and to stabilize reactive species. Among the possible alternatives, supramolecular metal-organic cages (GMOs) stand out for their versatility and relatively easy preparation. The inherent modularity of such supramolecular complexes potentially gives access to a remarkable diversity of GMOs.

In collaboration with experimental partners, the research aims at: i) developing new GMO-based complex catalysts, which possess distinctive chemical and electronic characteristics of the internal cavity suitable for applications in catalysis; ii) understanding the fundamental relationships linking cage structure, catalytic activity and selectivity, to the choice of metal centre(s) or ligand(s); ii) developing molecular models based on the use of advanced computational techniques for High Performance Computing (HPC) in order to identify GMOs with desired catalytic and selectivity properties.

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