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Metal-Organic Frameworks as advanced porous materials for gas separation and water remediation.

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The removal of contaminants from air and aquatic systems must be a priority research topic to re-establish ecosystem balance and secure a more sustainable future. In this context metal–organic frameworks (MOFs) have revealed them as excellent platforms for the removal of harmful species from both air and water. MOFs show great potential for applications in the area of environmental sustainability because their channels can be pre- or post-synthetically fine-tuned, in terms of size, shape, and functionality, resulting in a fascinating controlled host–guest chemistry. In addition, unlike other porous materials, MOFs allow for the use of X-ray crystallography to observe what happens within their channels. Single crystal X-ray diffraction leads to structural resolution that allows to understand and rationalize the adsorption mechanisms that conduct to an efficient capture or separation of hazardous species.
In this work, MOF-based technologies are reported unveiling successful developments achieved in the adsorptive removal of inorganic or organic contaminants. A new emerging class of porous materials, which are the mixed component metal-organic frameworks known as multivariate-MOFs (MTV-MOFs), have been also studied. In these MTV-MOFs heterogeneity and complexity are installed at the service of application performances. The modular nature of MTV-MOFs opens substantial possibilities in the field of water remediation, as it makes possible to tailor their porosity with two or more different and cooperative functional groups, capable of acting synergistically to capture contaminants of very different nature at once.
In-situ studies on single crystal X-ray diffraction by synchrotron radiation revealed the nature of the interactions of gases with MOF active sites. These results were used then to prepare rubbery mixed matrix membranes (MMMs) with MOFs as filler and new MMMs for liquid or gas phase capture/separation were produced and tested.

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