

The Importance of Metal-organic Frameworks in Today's World

Marcos Aurelio Gomes da Silva*

Professor and Researcher in the Areas of Natural Product Chemistry and Chemometrics and Bioenergy, Federal University of Juiz de Fora, Brazil

***Corresponding Author:** Marcos Aurelio Gomes da Silva, Professor and Researcher in the Areas of Natural Product Chemistry and Chemometrics and Bioenergy, Federal University of Juiz de Fora, Brazil.

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During the last few decades, research involving a new class of materials known as metal-organic networks (metal organic frameworks, MOFs) has developed at an extraordinary pace. These materials are constituted by an extensive network of metallic ions or clusters (clusters), coordinated to multidentate organic molecules, mostly carboxylates, bipyridines, sulfonates and phosphonates culminating in well-defined porous dimensions (FÉREY, 2011).

Metalorganic networks bring together relevant characteristics that make them unique, such as: high porosity, high internal surface area, presence of coordinately unsaturated sites, existence of strong metal-organic binder interaction, flexibility and ability to incorporate specific functionalities/active species without changing the topology of the framework (ROWSELL, 2004; ZHOU, 2008; VOGIATZIS, 2009).

These architectures have attracted a lot of attention due to their wide range of applications, such as gas purification, separation and storage (MURRAY, 2009; KUPPLER, 2010). Furthermore, they have high capacity as adsorbents and catalysts (FUJITA, 1994). Applications involving membranes, ultra-thin film devices, biomedical imaging, magnetic properties and non-linear optics (MATSUDA, 2005; TANASE, 2011) are increasingly gaining importance. Another advantage is due to their ability to act as molecular sieves, specifying how molecules can diffuse into pores.

Thus, these materials have interesting physicochemical properties and potential to be used in economically viable applications, filling a gap between surface non-porous

organometallic catalysts, microporous zeolites and mesoporous silicates.

The study in the area of metal-organic networks has the collaboration of the Dynamique & Adsorption dans les Matériaux Poreux (DAMP) group, headquartered at the Charles Gerhardt Institute of the Université de Montpellier 2 (UM2). Several materials are being studied in order to investigate the interactions present in the adsorption of molecules, as well as to verify the stability of the material under moisture through the minimum energy path (MEP) for the dissociation reaction of the water molecule. The figure below shows the energy barriers in kJ/mol for the dissociation reaction of 1 molecule of water in the porous cavity of MIL-140^a.