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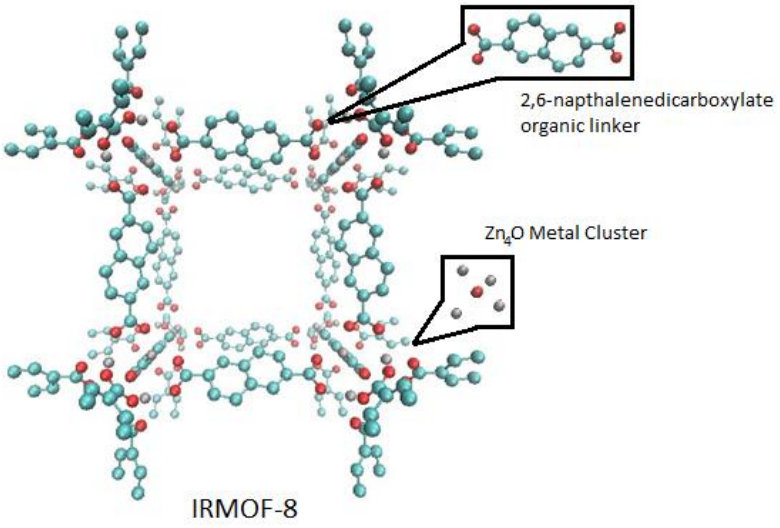
Metal Organic Frameworks and Gas Storage

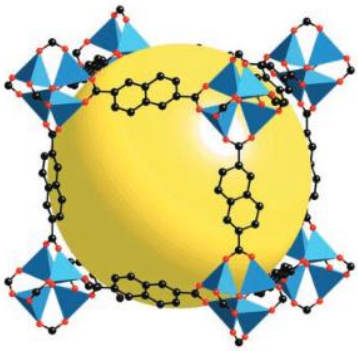
Metal organic materials (MOMs) are materials comprised of inorganic metal clusters joined by organic linkers. Nearly any transition metal can be used as a cluster and the number of organic linkers available is immense. As such, the current number of documented MOFs that have been reported and studied is approaching 55,000. (University of Cambridge, 2015) Each MOM is organized in a way that it can be replicated and attached to other copies of the same MOM in a crystalline manner. When MOMs are built into a three dimensional shape, they are referred to as metal organic frameworks (MOFs).

The image to the right shows IRMOF-8, an isoreticular MOF comprised of a Zn_4O metal cluster and a 2,6-napthalenedicarboxylate. This MOF has an equilateral side length of 30.0915 angstroms. Due to the cubic structure, it is able to be arranged into a cubic crystalline framework.

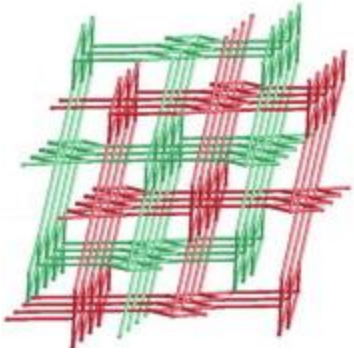


Metal organic frameworks share several basic characteristics with each other. MOFs typically have a large surface area which exceeds other porous materials such as zeolites. Additionally, MOFs are highly porous, often times having a porosity of more than 50% of the crystal volume. (Furukawa, Cordova, O'Keeffe, & Yaghi, 2013) MOFs are also chemically and thermally stable as well as having the ability to have their size and nature changed based on the metal cluster or organic linker used. Due to

these properties, metal organic frameworks have several promising uses being explored. Uses at the forefront of current research include catalyzing organic reactions, biomedical imaging, small particle conduction, gas separation, and gas storage.



Due to the high porosity of metal organic frameworks, they have been proven to be highly efficient as gas storage for certain sorbates, particularly hydrogen and carbon dioxide. The image to the right shows the largest molecule that can be held by IRMOF-8 without interfering with the van der waals interactions of the MOF. The size of the sorbate can be changed based on the linker used. If a longer linker is used, a larger sorbate can be held. A fine line exists between allowing more room for the largest sorbate possible and negative results from large unit cells. The more space available within the MOF, the more likely it is to interpenetrate; that is to link together with another MOF and intertwine with it permanently. The image to the right depicts two interpenetrated MOFs, shown in red and green. The metal clusters of each MOF reside in the pores of the other MOF, decreasing each MOFs porosity greatly. Interpenetration of MOFs leads to a decreased porosity and therefore a decrease in ability to sorb molecules.



A key use for metal organic frameworks is gas storage, particularly for energy use. The United States Department of Energy has set a target for on-board vehicle H_2 storage of 5.5 wt % at a temperature of -40°C to 60°C under pressures of no more than 100 atm. While this target has not yet been met, advances in MOF technology have led to prototype vehicles being produces with MOF based hydrogen storage cells for energy use. At present time, the sorbtion of hydrogen in metal organic frameworks is excellent at high pressure and low temperature but are decreases at ambient

temperature and pressure. (Suh, 2011) Research continues in an effort to meet and exceed the Department of Energy standards.

References

Furukawa, H., Cordova, K., O'Keeffe, M., & Yaghi, O. (2013). The Chemistry and Applications of Metal-Organic Frameworks. *Science*, 341.

Suh, M. P. (2011). Hydrogen Storage in Metal-Organic Frameworks. *Chemical Reviews 112.2*, 782-835.

University of Cambridge. (2015). *Cambridge Crystallographic Data Centre*.