# Metal Organic Frameworks for Atmospheric Water Harvester

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#### Overview

Scarcity of pure drinkable water has made many researchers think of new alternative techniques for harvesting water from the environment. In the quest for new sources of pure water, researchers have invented many technologies involving seawater sweetening and water cultivation from the air. Desalination of seawater is expensive and also there is an issue of sludge management whereas, water harvesting from moist air is less expensive and it has no issues of sludge <sup>[1]</sup>. Among many technologies, the environment-friendly adsorption based water harvesting system stands out as an emerging future technology due to its low power consumption<sup>[2]</sup>. Metal organic frameworks (MOFs) are thought to be the next generation adsorbents for water based adsorption systems due their regular structure, tunable porosity and most importantly their water adsorption isotherm's shapes<sup>[3]</sup>. This study focuses on the synthesis and characterization of two porous metal organic frameworks- MOF 801 and MIL 100 (Fe) intended for the application of adsorption based water harvester.

# Synthesis of metal organic frameworks

MOF 801 is a microporous 3D framework having zirconium (Zr<sub>6</sub>) nodes bridged with fumarate linkers<sup>[4]</sup>. To synthesize this ZrOCl<sub>2</sub>·8H<sub>2</sub>O and fumaric acid (having the ratio of 1:0.36 in terms of gm) was dissolved in a solvent made of DMF and formic acid (1: 0.35 in terms of liter). Then the mixture was heated at 130 °C for 6 hours and MOF 801 precipitated. Then the synthesized MOF 801 was separated, washed, dried and then activated by heating at 150 °C inside the vacuum.

In case of MIL 100 (Fe), the molar ratio Fe : BTC :  $HNO_3 : H_2O$  of 1: 0.67 : 0.60 : 166 was used for the hydrothermal synthesis<sup>[5]</sup>. All reactants were mixed and loaded into a Teflon autoclave which was heated at 150 °C for 12 h. The resulting MIL-100(Fe) solid was collected and washed for several times using distilled water. Subsequently, the MIL-100(Fe) solid was purified by soaking in water at 80 °C for 1 h, followed by ethanol at 60 °C for 3 h. The purified MIL-100(Fe) was dried in a 60 °C oven and heat-activated using a vacuum oven for 2 h at 120 °C.

## Material characterization

 $N_2$  adsorption was done on both the samples at 77K to investigate about their BET surface area and pore size distribution. The results are furnished in Table 1. FESEM was done on both the samples to examine their morphological depiction. The water uptake was also measured for both the MOFs using thermos-gravimetric analyzer.

## **Results and discussion**

Table 1 shows that MIL 100 (Fe) has significantly higher surface area and pore volume when compared with MOF 801. The pore size distribution of the two assorted MOFs are shown in Fig 1 (a) and (b) respectively. We can conclude that both the samples are highly microporous. FESEM images of the two MOFs are depicted in Fig 1 (c) and (d) respectively. MOF 801 has regular circular shaped grains where for MIL 100 (Fe) the grains were irregular in shape. The water uptake for both the samples are exhibited in Fig 2 (a) and (b) at 303 K. It is evident that MIL 100 (Fe) has higher water uptake than MOF 801. However, MOF 801 has high uptake in the lower relative pressure region (less than 30 % RH).



Fig. 1 Pore size distribution of (a) MOF 801, (b) MIL 100 (Fe); FESEM image of (c) MOF 801, (d) MIL 100 (Fe)



Table 1. porous properties of MOF 801 and MIL 100 (Fe)

#### Conclusions

MIL 100 (Fe) MOF had higher surface area and pore volume than MOF 801. Hence MIL 100 (Fe) higher water uptake in saturation pressure when compared with MOF 801. However, MOF 801 has steeper water uptake in low pressure region ensuring its applicability in water harvesting in the desert areas of the world while MIL 100 (Fe) can be used in the tropical regions. Again using MOF 801 an multiple cycle adsorption based atmospheric water harvester is possible where as in case of MIL 100 Fe there will be only one cycle as the high humidity of 35% or more can only be achieved in the night times. On the other hand MIL 100 offers an advantage over MOF 801 in case of regeneration temperatures. MOF 801 requires to be regenerated until it bed reaches a vapor pressure of 10% RH or less where for MIL 100 Fe the requirement is only until 20%-25% RH.

# Reference

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