

## **Applications of adsorption in atmospheric water harvesting**

There is an increasing understanding of the climate changes, and the possible water shortage. A global problem of water scarcity will affect most of the world's population, half of which will live in water-stressed areas after 2030. Water harvesting from atmosphere is one of the envisaged solutions which can be applied in many situations: it is a promising strategy for decentralized water production, without the long-distance transport, delivery of potable water in rural areas and, of course, in the situation of water scarcity of arid regions. The advancement of additional methods for freshwater generation is imperative to effectively address the possible global water shortage crisis. In this regard, extraction of the ubiquitous atmospheric moisture is a powerful strategy allowing for decentralized access to potable water. The energy requirements as well as the temporal and spatial restrictions of this approach can be substantially reduced if an appropriate sorbent is integrated in the atmospheric water generator.

As climate change causes drought to intensify in dry areas and global water use continues to increase. There are some technologies, suitable for large-scale centralized production due to their high capital cost, such as membrane and thermal desalination which already provide water in many areas of the globe. However, a decentralized water production is an important strategy for rural populations or in areas where economies do not favor centralized networks approach. Atmospheric water harvesting (AWH) presents a potential solution in areas where liquid water is or will become physically scarce. It can also offer a general use solution, in which infrastructure and water for consumption are physically isolated from contaminated water supplies.

This project aims at fundamental understanding of the water adsorption mechanism in nano-porous materials from the perspective of applications as the adsorbent in the water harvesting from atmosphere. The choice of the porous structures is critical. The applications of zeolites and silica gels suffer from relatively low adsorption uptake which naturally eliminates them from efficient use. Metal-organic frameworks (MOFs) porous ordered systems are novel crystalline materials which properties make them potentially interesting for the future applications. Their combinatorial architecture, which consists of inorganic nodes (metal ions, clusters, or chains) and organic linkers, allows for design and synthesis of almost unlimited number of structures. Remembering that there are already more than hundreds of thousands of MOFs structures, it is crucial to precisely define which structural microscopic properties are essential for an effective water adsorption.

Currently, there are three separate categories of AWH: fog harvesting, dewing, and sorption-based approaches. Fog harvesting uses large nets to capture small water droplets that are suspended in the air. Dewing refrigerates the air below the dew point to condense water vapor. Both of them use traditional, macroscale technologies. Sorption-based approaches uses a nano-porous systems to harvest water from the atmosphere and shows much bigger potential for efficient applications. To achieve this goal, the mechanism of adsorption must be very well understood.

In this project, we focus on nano-porous solid adsorbents for water harvesting. Metal-organic frameworks (MOFs) porous ordered systems will be studied, in particular, a possibility to of using the MOFs flexibility will be explored. The methodology is both numerical and experimental, where the mechanism of water adsorption will be numerically modeled and simulated, then the experimental measurements will serve as the verification tools. The main expected result will propose a model ideal adsorber for the AWH applications.