Advanced methods of numerical modeling supported by machine learning tools for predicting water adsorption in MOF materials

Passive adsorption-based atmospheric water harvesting (Figure 1) has great potential for decentralized drinking water supply in many arid regions of the world. The method involves the adsorption of water molecules from the atmosphere onto a porous material and then, by changing the operating conditions (e.g., by heating), desorption, and condensation, obtaining water in a liquid state. This requires suitable adsorbents (i.e., materials on whose surface adsorption takes place), which can be tailored to achieve the maximum values of the operational capacity, the expected isotherm shape, or the relative pressure values at which adsorption and desorption occur. Considering these factors, materials from the group of metal–organic frameworks (MOFs) are very promising, mainly due to their structural diversity, as well as their designability and functionalization possibilities. The total number of synthesized MOF structures is difficult to estimate – for example, the CSD MOF database contains a striking number of ~100,000 structures. Given this value, computational research using the most efficient simulation techniques plays a key role in the search and discovery of new materials.

The aim of this project is to **characterize, develop, and use an efficient and accurate molecular modeling algorithm, supported by machine learning tools, to perform water adsorption screening of available metal-organic frameworks (MOFs) with potential applications as adsorbents in atmospheric water harvesting systems.**

The most important expected outcome of this project will be the identification of several potential MOF structures that have the best characteristics for use in atmospheric water harvesting. These structures will be synthesized, and their adsorption capacity will be verified experimentally. In addition, side results that are crucial for the development of nanoengineering should be identified, such as the development of molecular modeling methods for water adsorption, the creation of an ideal water adsorbent model that can be used for the design of new materials or a better understanding of water adsorption in porous materials.

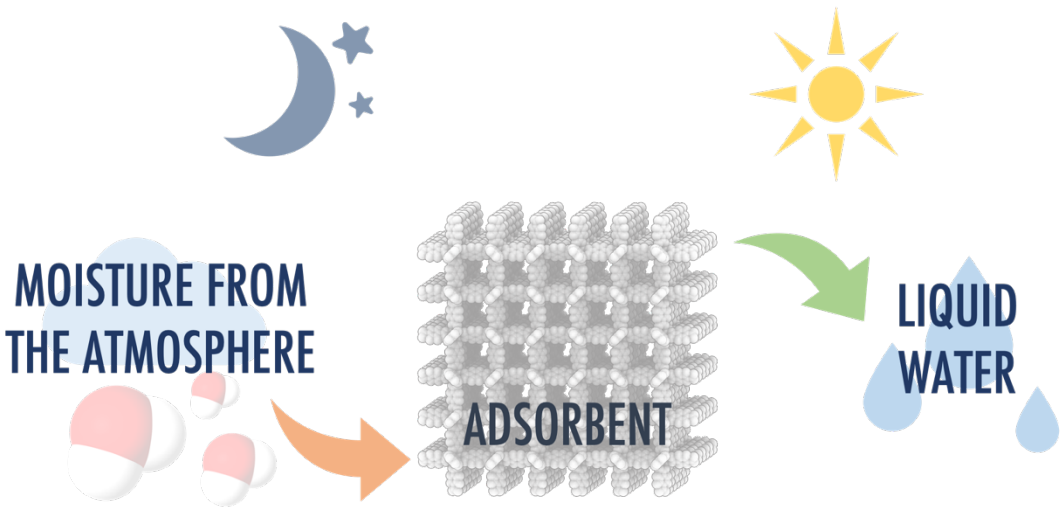

Figure 1. Schematic representation of an atmospheric water harvesting device.