Water Independence for People Everywhere: Scaling up Next Generation MOFs and Water Harvesters

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Aims and Objectives

The project aims to accelerate the discovery of high-uptake capacity metal-organic frameworks (MOFs) using Generative AI and Robotics as well as to build passive (i.e., no electricity requirements), portable, scalable modules capable of generating from air 2 Liter (Harvester**Mini**) and 20 Liter (Harvester**Pro**) of water each day. These modules will work anywhere in the world at any time of the year regardless of weather conditions. An education program to engage emerging scholars from Europe will train one postdoctoral fellow and three visiting students during the 3-year period.

Background

Water scarcity is predicted by the United Nations to be one of the most pressing issues of the 21st century with over five billion people expected to be affected by it by the year 2050 [1]. As we write, nearly half a billion people in the world are facing severe water scarcity all year round, most of them in developing countries that significantly lack water supply infrastructure [2]. Given that the atmosphere holds as much fresh water as there is in all the lakes and rivers combined on our planet, it is natural to tap into this resource and harvest the water to satisfy our needs. We have developed different devices based on porous reticular materials, both active [3], and passive [4, 5, 6, 7], to harvest water from the atmosphere. We wish to take this to the next level by scaling it to capture and deliver higher and higher amounts of water within the smallest footprint, minimal energy input, and lowest cost.

The scaled-up water harvesting module: challenges to address

At its core, any water harvesting device likely uses a porous material such as a metal- organic framework (MOF) that can adsorb water from the atmosphere, and when heated, releases the water vapor that is then collected by condensation.

Uptake capacity: We recently developed a MOF material which takes up 50% more than our previous water uptake record. In the next step, we would like to discover even better materials with the help of generative AI and robotics.

Desorption temperature: This new MOF is also able to release water under mild conditions only requiring ambient heating by sunlight.

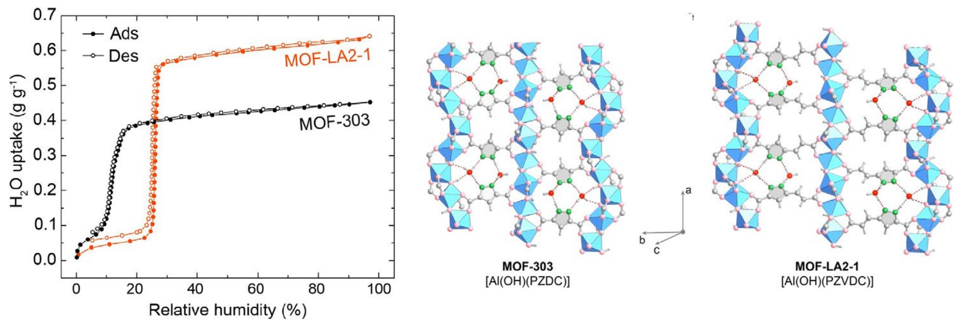
Adsorption-desorption cycle time: An important step that takes a significant amount of time during a given cycle is the desorption step. In this step, the MOF is enclosed and heated to a temperature that allows for the water vapor to be released from the pores of the MOF, and evaporate, encountering a condenser, where it condenses. Reaching this temperature using natural sunlight is time-consuming. We will address this challenge in our new water harvester design.

Increasing the number of cycles per day: Another major bottleneck to increasing the water production output from a passive device is to find a way of increasing the number of cycles that can be performed per day without any external energy input - this is challenging since to run multiple cycles, the MOF must be (i) exposed to the air for the adsorption cycle, and then (ii) be enclosed in a closed area, to allow for the desorption cycle, where the MOF is heated and the water vapor is released, to take place. Both these steps have to take place one after the other in a cyclical manner; for this to be possible there has to be a mechanical barrier that can open, which allows the MOF to be exposed to the air, and then closed, which allows the MOF to be heated, to allow for the desorption of the water vapor.

Accelerating the discovery of high-uptake capacity MOFs using Generative AI and Robotics

We aim to leverage the capabilities of generative AI, particularly fine-tuned large language models (LLMs), to accelerate the discovery and design of novel linkers for metal-organic frameworks (MOFs) with enhanced water uptake properties. Recent advances in AI- driven material design have demonstrated the potential of LLMs to suggest, edit, and optimize linker structures, which could be tailored to improve water adsorption capacities in MOFs [8]. Using a carefully curated dataset, we will fine-tune our LLM to understand key chemical features associated with high water uptake, such as pore size, hydrophilicity, and binding site density. To further enhance our workflow, we propose to integrate robotic systems for automated synthesis and high-throughput characterization of the AI-designed linkers. This robotic platform will enable rapid, reproducible synthesis and real-time evaluation of each MOF's performance under controlled conditions, ensuring a seamless feedback loop between design, synthesis, and testing.

By combining AI-assisted linker design with automation, we aim to systematically explore a vast chemical space, identifying MOFs that not only exhibit superior water harvesting capabilities but also demonstrate efficiency in adsorption and desorption cycles. This integration of generative AI with robotics-driven synthesis and characterization will allow us to push beyond current benchmarks in water harvesting, achieving both high capacity and operational efficiency. The figure below shows the water adsorption isotherm of two key MOFs at 25 °C along with their formula and structures: Al, blue octahedron; C and H, gray; N, green; O in framework, pink; O in H_2O, red. The details are outlined in the next section.



Water Harvester Parameters

The proposed design is inspired by certain types of flowers that can open and close in response to external stimuli - importantly, the design will address the issues outlined above. At the core is the MOF cartridge which contains discs of MOF that capture water from the atmosphere. The current benchmark material for water harvesting has been shown to deliver about 0.250 Liter of H_2O per kilogram of MOF-303 per cycle without any power or energy input aside from ambient sunlight [7]. Recently, a newly discovered MOF, MOF-LA2-1, has been shown to deliver 50% higher water capacities as compared to MOF- 303 [9]. Changing the type of MOF in the cartridge from MOF-303 to MOF-LA2-1 will allow us to increase the water harvesting capacity to about 0.375 Liter of H_2O per kg of MOF per cycle using the existing device alone. In this proposal we will reach the target of 1 Liter of H_2O per kg of MOF per cycle.

The device has been designed keeping in mind the three key design principles we started with: portability, modularity, and scalability. On the top of the device is a solar panel, which charges the batteries. The batteries are critical for the operation of the inner and outer cylinders/double clamshells.

Expected Performance Characteristics and Technical Specifications

The following assumptions underlie an estimation of the expected performance of the next generation water harvester:

The performance characteristics of the proposed device are at a minimum equivalent to those obtained for the passive water harvesting presented in the work by Song, Yaghi et al. [7] and hence many of the performance metrics can be extrapolated for the system considered in this proposal. We consider the duration of a 24-hour cycle where daylight runs from 7 a.m. to 5 p.m., while from 5 p.m. to 7 a.m. (next day) there is no sunlight. The temperature is considered to be near 25 °C with a maximum of 40 % RH environment. Cumulatively, we should be able to harvest nearly 1 Liter of water per kg of MOF in 24 hours, i.e., a total of 3 adsorption-desorption cycles. The next challenge is to then find a way of maximizing the amount of MOF that can be enclosed within the device, and this is where the density of the MOF becomes important. For MOF-LA2-1, we make conservative estimates: ~ 0.50 g cm^{-3} (the calculated density from the crystal structure is 0.847 g cm^{-3}), taking into account that on adding binder there will be a certain degree of reduction in the usable porosity of the MOF. We consider a cylinder/MOF cartridge of diameter equal to 0.2 ft and height equal to 2 ft with a usable volume of ~ 2300 cm^3. Here, it is important to note that a certain volume of space must be left 'open' to allow for the air to flow through and access all the porosity of the MOF. We allocate ~ 300 cm^3 of volume for this purpose, leaving us with ~ 2000 cm^3 to pack the MOF. This way we will be able to pack ~ 1 kg of MOF and extract ~ 1 L of water per day from a 2 ft device. Given that our design is scalable, we also expect to be able to provide 4 ft x 0.5 ft device with water harvesting capacities of 2 Liter per day.

Proposed Size Options for Water Harvesters, their productivity, and properties

We propose two options:

Option 1 – Harvester**Mini**: A module sized 4ft x 0.5 ft weighing at least 4 kilograms, delivering 2 Liters of water per day (Note: 2 kilograms of MOF). This is a personalized unit which could be multiplied to provide higher amounts of water (e.g., 10 HarvesterMini will deliver 20 L of water). For this larger amount of water, we propose an alternative option.

Option 2 – Harvester**Pro**: A single module sized 4 ft x 3 ft weighing about 30 kilograms, delivering 20 Liters of water per day (Note: 20 kilogram of MOF). This is a family-size unit which could also be multiplied to provide higher amounts of water (e.g., 10 HarvesterPro will deliver 200 Liters of water per day).

The MOF remain in the device for at least 5-6 years without requiring maintenance. At the end of the MOF lifetime, it can be disassembled and reassembled using water-based methods and without discharging any waste. The water generated using the module is 100% pure, and after being passed through a small mineralizing cartridge, it becomes drinkable.

Education of Emerging Scholars from Europe

We intend to include undergraduates, graduate students, and postdoctoral scholars in the various activities proposed for the discoveries of water-harvesting MOFs and the design of two water harvesters for the Balzan Research Projects. Specifically, we hope to train one postdoctoral fellow for three years. This researcher will be involved in and oversee the carrying out of the research objectives proposed here. In addition, three visiting students, one for each of the three years and for the duration of 6-12 months, will be mentored by the Balzan postdoctoral fellow and Prof. Yaghi on the materials discovery research using generative AI and robotics. Preference is given to young European scholars. These scholars will have opportunities to participate in the modeling/AI work, Synthesis, and characterization of MOFs, as well as building the devices. The specific major tasks the scholars will be developing are listed here:

1. Computation: It will be necessary to carry out DFT computation on the MOF structure to determine its humidity cut-off and overall capacity. Engineering of the device will require modeling of air movement, mass transport, energy requirements, and temperature variation across the MOF during operation. This is necessary for optimizing water output at the highest energy efficiency.
2. Chemical synthesis and characterization: The project will employ robotics techniques to explore the MOF synthesis space. Once the MOF is identified it will be scaled up to kilogram quantities and fully characterized by spectroscopy, diffraction, and gas adsorption techniques.
3. Water harvester device development: This task requires making MOF coatings and the MOF discs to be placed into the device. The device construction will be iterative and will go hand in hand with the modeling described in point 1.

The participating scholars will gain a gamut of experiences ranging from the basic science of MOF and synthesis to characterization of porosity and solid-state materials, ultimately developing the very devices which will incorporate the water harvesting MOF. Time permitting, these water harvester devices will be tested in the desert.

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