Master thesis

Water production from thin air: Energy efficient designs for adsorption-based atmospheric water harvesting (AWH) using metal-organic frameworks (MOFs)

Atmospheric water, in the form of water vapor and droplets in the atmosphere, is an alternative natural water resource equivalent to ~14% of all freshwater in the lakes on Earth. Therefore, it has great potential to tackle water scarcity problems. Among different atmospheric water harvesting methods, sorption-based techniques recently gathered scientific attention with the development of metal-organic frameworks (MOFs). MOFs are a new class of chemically tunable high uptake porous nanomaterials wherein large amounts of specific gas species (e.g. water vapor) can be adsorbed, stored and released for further use. Water vapor is initially adsorbed by the MOFs at ambient conditions and then heat (e.g. solar thermal, waste-heat) is supplied to release the captured water. The surrounding air is thus humidified in order to allow condensation of water vapor at energetically favorable temperatures. However, the productivity of MOF-based AWH (passive solar thermal or cyclic) is limited to on the order of 0.1-2 L/day despite the performance metric (e.g. $L/kg_{MOF}/day$ or $L/m^2/day$). The reason for this deficiency is the lack of scalable designs and robust porous MOF form factors compatible with rapid mass and heat transport.

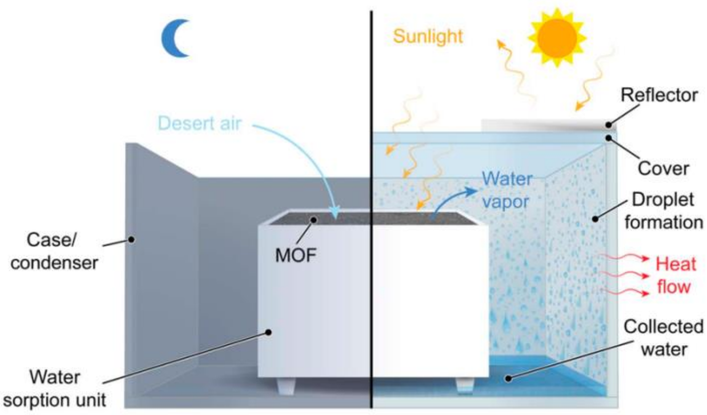

Figure: Example of an atmospheric water harvester operating in a single daily cycle. Water vapor is adsorbed during night-time and solar heat is supplied during day-time to release the captured water in a controlled volume box. Image from *Science Advances 4, eaat3198 (2018)*. In this master project, multi-cyclic operation designs will be explored in order to increase dramatically the daily water productivity. Further, the goal is to liquify water at ambient dewpoints (no extra chiller is needed).

In MOF-based AWH, multiple transport processes occur, and over different length scales. These include adsorption-desorption dynamics within single MOF crystals (*nanoscale*), mass, momentum and energy transport in the interstitial spaces between the MOF grains, i.e. porous agglomerates (*microscale*), or exchange processes between the global porous MOF form factor and the surrounding air (*macroscale*). However, our understanding of many of these physical phenomena in MOF-based systems is still at a nascent state. The **motivation** for the proposal is thus to promote these advancements and provide a fundamental knowledge to build on toward atmospheric water harvesting with productivity rates matching human consumption. In particular, the project **aims** to quantify multi-field processes (mass, momentum and energy transport) in porous MOF-based systems, and employ this knowledge for the development of a novel atmospheric water harvester design operating at ambient dewpoints (no extra chiller is needed).

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