

# MOF water harvester produces water from Death Valley desert air in ambient sunlight

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## Supplementary Methods

### *Chemicals*

The chemicals were purchased from the following companies and used without further purification: methanol and dichloromethane (Acros Organics), 3,5-pyrazoledicarboxylic acid (H<sub>2</sub>PDC, ChemScene), aluminum chloride hexahydrate (AlCl<sub>3</sub>·6H<sub>2</sub>O) and sodium hydroxide (ThermoFisher Scientific), PTFE (powder form, 1 μm), carbon nanofiber (100 nm × 20 – 200 μm, Sigma-Aldrich), and cellulose binder (SPEX), Graphite (Merck, cat#: 1042062500).

### *Analysis of MOF-303 powder and MOF-graphite pellets*

Powder X-ray diffraction (PXRD) spectra were collected using a Rigaku Miniflex 600 diffractometer with focused radiation source of Cu K $\alpha$  line ( $\lambda = 1.5418 \text{ \AA}$ ) at 600 W (40 kV, 40 mA). N<sub>2</sub> BET surface area measurements were performed using an ASAP 2420 accelerated surface area and porosimetry analyzer (Micromeritics). Fourier-transform infrared (FT-IR) spectra were measured using Alpha II compact FT-IR spectrometer equipped with an ATR module (Bruker).

### *Water uptake evaluation of the MOF cartridge*

The MOF cartridge assembly was first activated in an oven at 140 °C for 24 hours. The cartridge was incubated in the environmental test chamber (ESPEC, SH-242) under the controlled temperature and humidity (25 °C and 40 % RH) conditions. The weight of the cartridge was intermittently measured to observe the time-dependent water uptake properties.

### *Radiative, conductive, and convective energy transfer simulation of the device under solar irradiation.*

To investigate the potential of effective solar heating of the device as well as heat dissipation to the environments, COMSOL simulation was performed. The device geometry was imported from Solidworks throughout the Parasolid file format. The Surface-to-Surface Radiation (rad), Heat Transfer in Solids and Fluids 2 (ht2), and Laminar Flow (spf) modules were used for the simulation, coupling the (rad) and (ht2) modules by Multiphysics. Followings are the simulation parameters and boundary conditions: external radiation source (5000K, 1000W/m<sup>2</sup>), internal device space as weakly compressible air (gravity included), ambient temperature (25 [degC]), heat flux to ambient (convective heat flux,  $h = 15 \text{ W/(m}^2\cdot\text{K)}$ ), MOF housing (transparent for solar spectral band and opaque for ambient spectral band).

**Scanning electron microscopy (SEM).** SEM images were obtained on an FEI Quanta 3D FEG scanning electron microscope with an accelerating voltage of 10 kV and a working distance of 10 mm. The samples

were dispersed on carbon tape on a stainless-steel holder.

***Maximum specific yield ( $SY_{water,max}$ ) of water and device efficiency ( $\eta$ ) calculations***

$SY_{water,max}$  of sorbent-assisted passive atmospheric water harvesting (AWH) device is maximum amount of liquid water that can be extracted from air at given conditions and energy input.

$$SY_{water,max} = \frac{L_{max}}{P_{total}} \quad (1)$$

where  $L_{max}$  (L/h) and  $P_{total}$  (kW) are maximum water production rate during the day cycle and minimum energy required to desorb all water from adsorbents, respectively.

$$L_{max} = \frac{\text{Maximum amount of water that can be sorbed during night cycle (L)}}{\text{Operation time of day cycle (h)}} \quad (2)$$

$$P_{total} = \left( \Delta H^{des} + C_{p,w}(T_{des} - T_{amb}) \right) L_{max} \quad (3)$$

where  $\Delta H^{des}$  is energy required to desorb water,  $C_{p,w}$  is heat capacity of water,  $T_{des}$  is desorption temperature, and  $T_{amb}$  is ambient temperature. In this study, maximum amount of water that can be sorbed during night cycle in equation (2) was obtained from water uptake isotherm and average relative humidity (RH) of each field test during the night.  $\Delta H^{des}$  is the same as isosteric heat of adsorption and 52 kJ/mol (2888 kJ/kg) is used<sup>1, 2</sup>. Average temperature of MOF housing and ambient air during the day cycles of each field test were adopted as  $T_{des}$  and  $T_{amb}$ , respectively.

The device efficiency ( $\eta$ ) is defined as equation (4).

$$\eta (\%) = \frac{SY_{water}}{SY_{water,max}} \times 100 \quad (4)$$

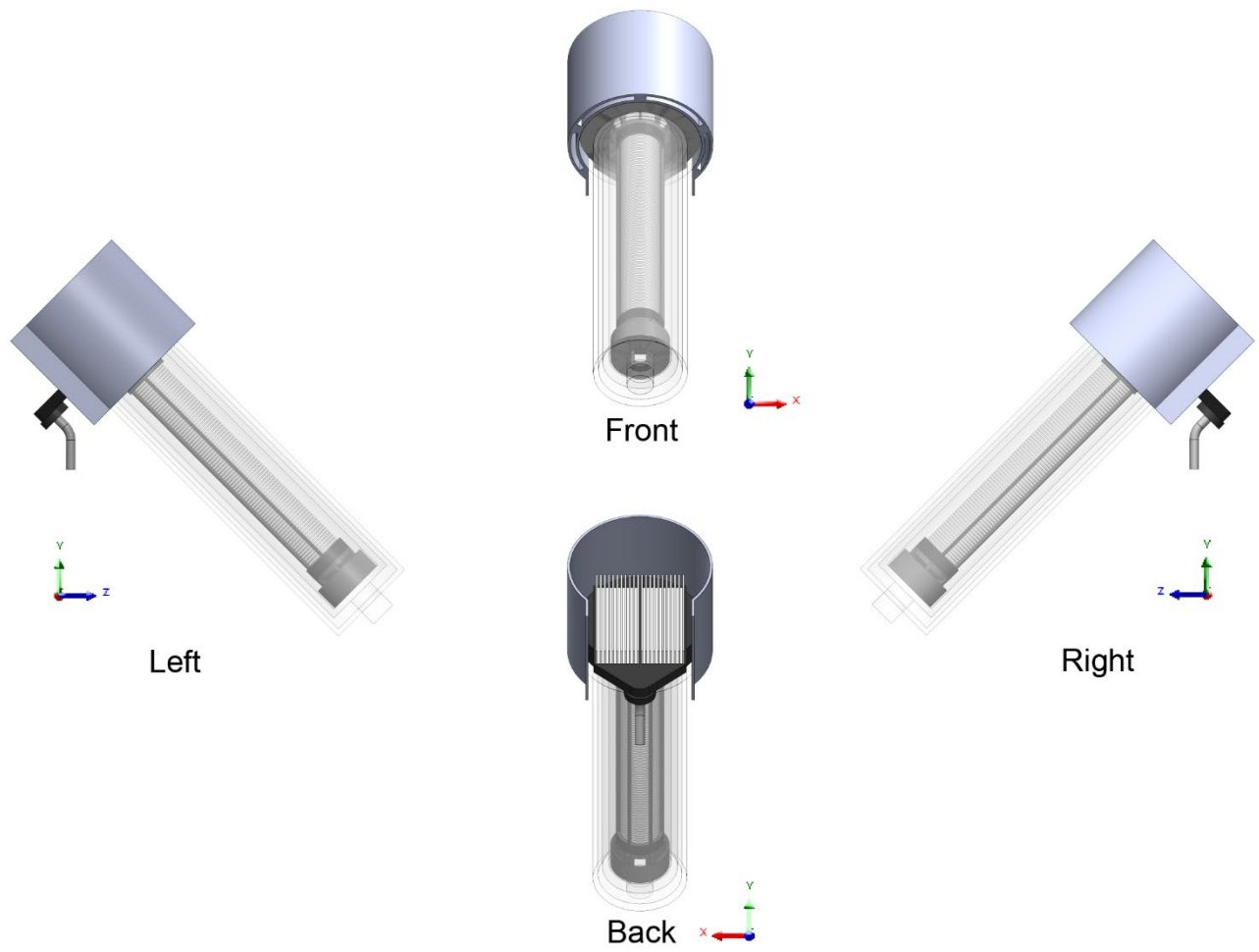
where  $SY_{water}$  is actual specific water yield of the device tested in the field.  $SY_{water}$  is defined as equation (5).

$$SY_{water} = \frac{L_{actual}}{P_{input}} \quad (5)$$

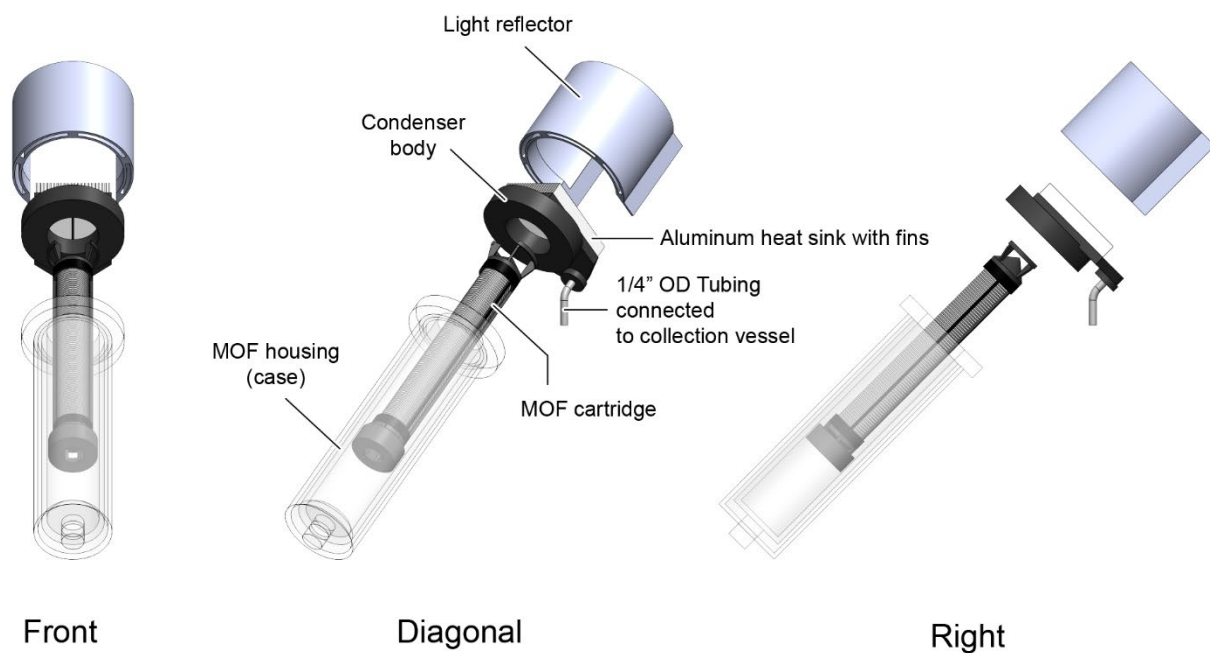
where  $L_{actual}$  (L/h) and  $P_{actual}$  (kW) are actual water production rate of the device during the day cycle and energy used to desorb that water from adsorbents, respectively.

$$L_{actual} = \frac{\text{Water harvested (L)}}{\text{Operation time of day cycle (h)}} \quad (6)$$

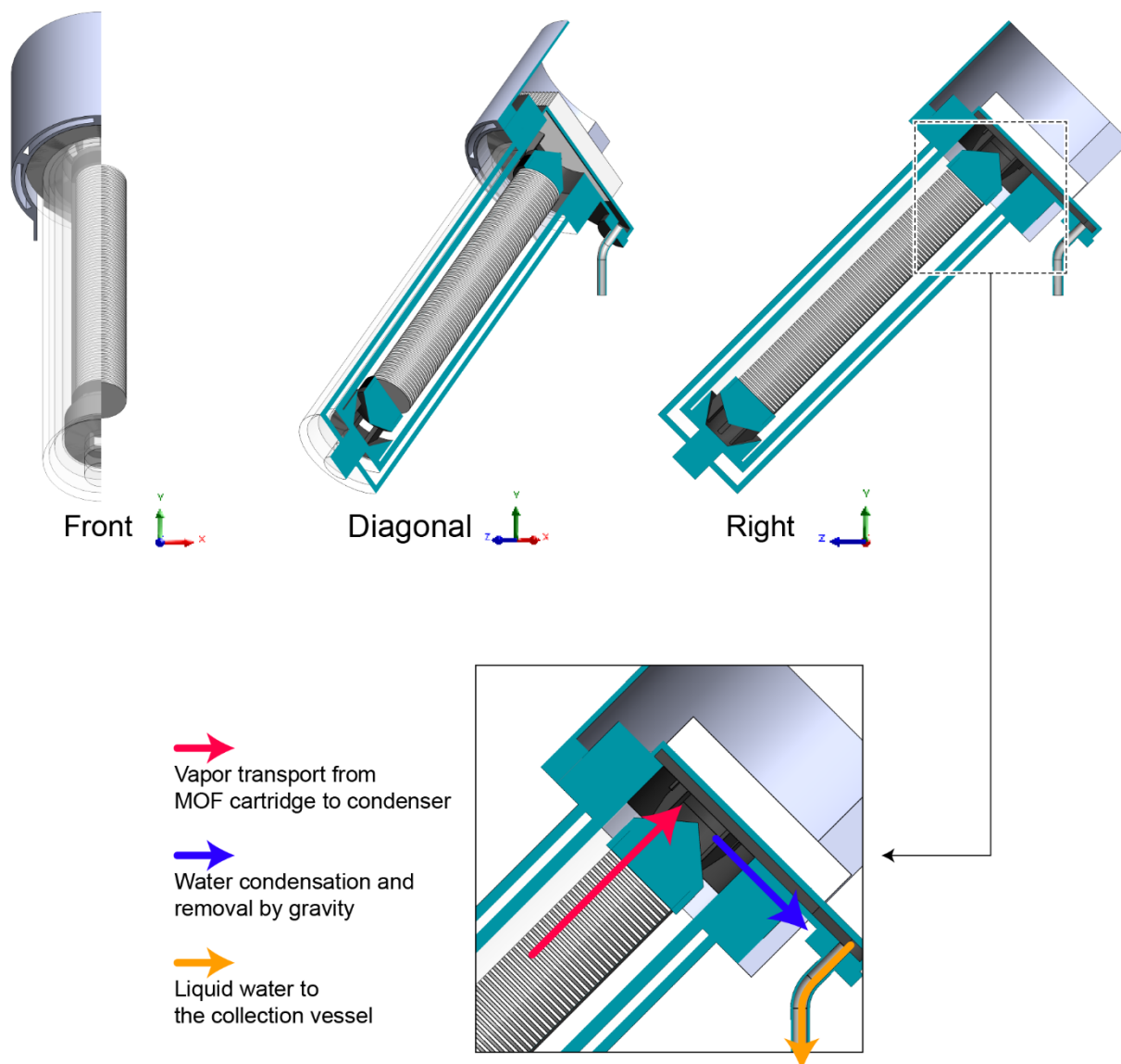
$$P_{total} = \left( \Delta H^{des} + C_{p,w}(T_{des} - T_{amb}) \right) L_{actual} \quad (7)$$



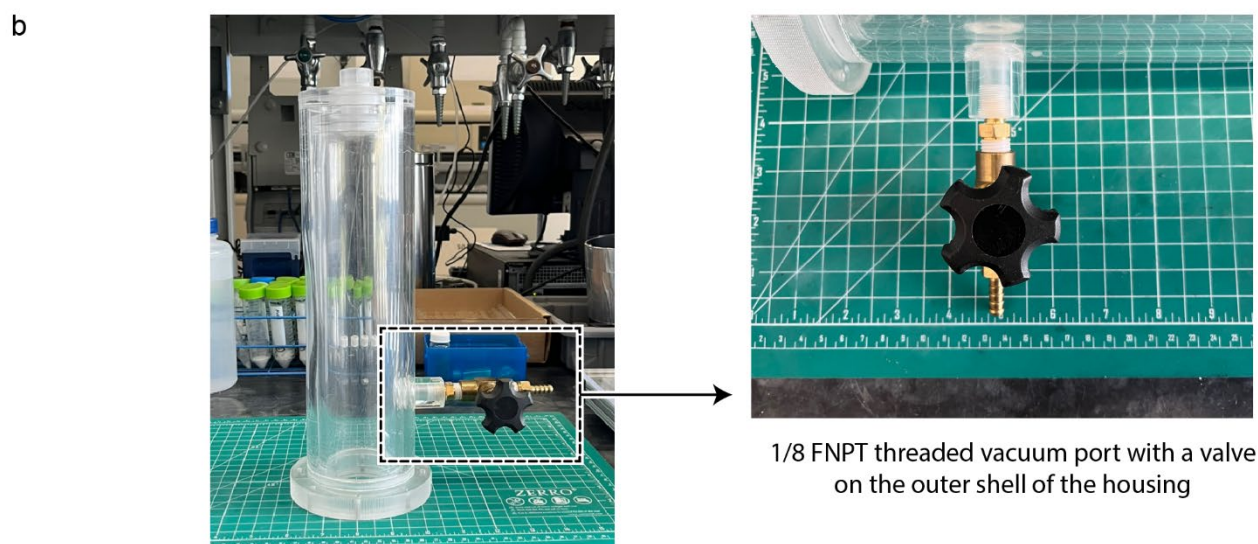
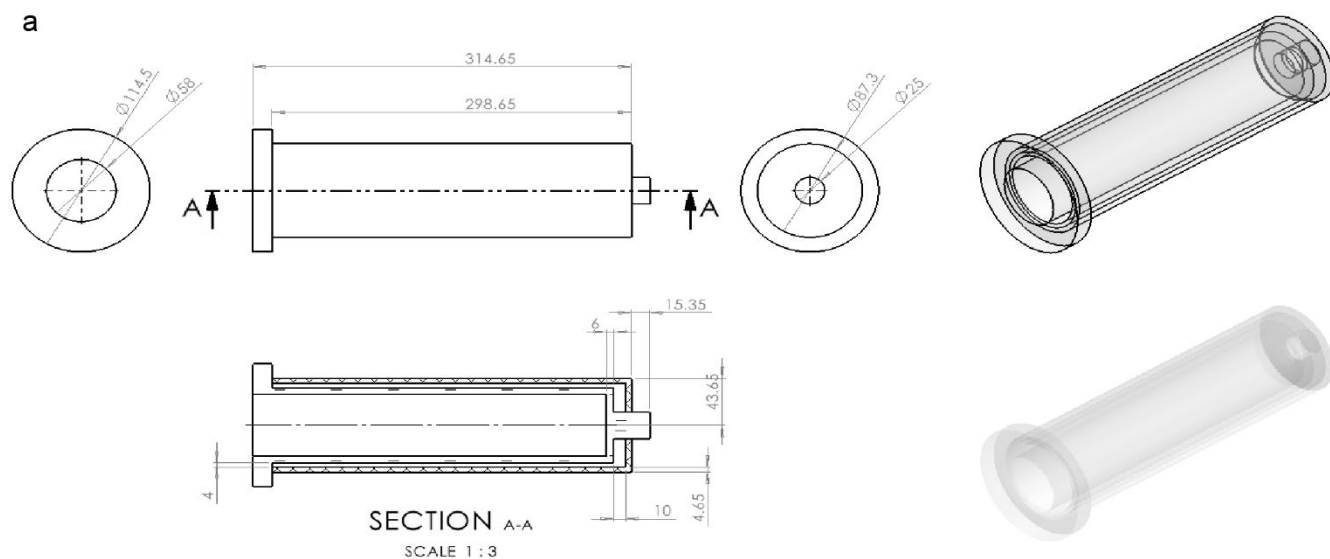
**Supplementary Fig.1.** 3D Drawings of the device structure with different views.



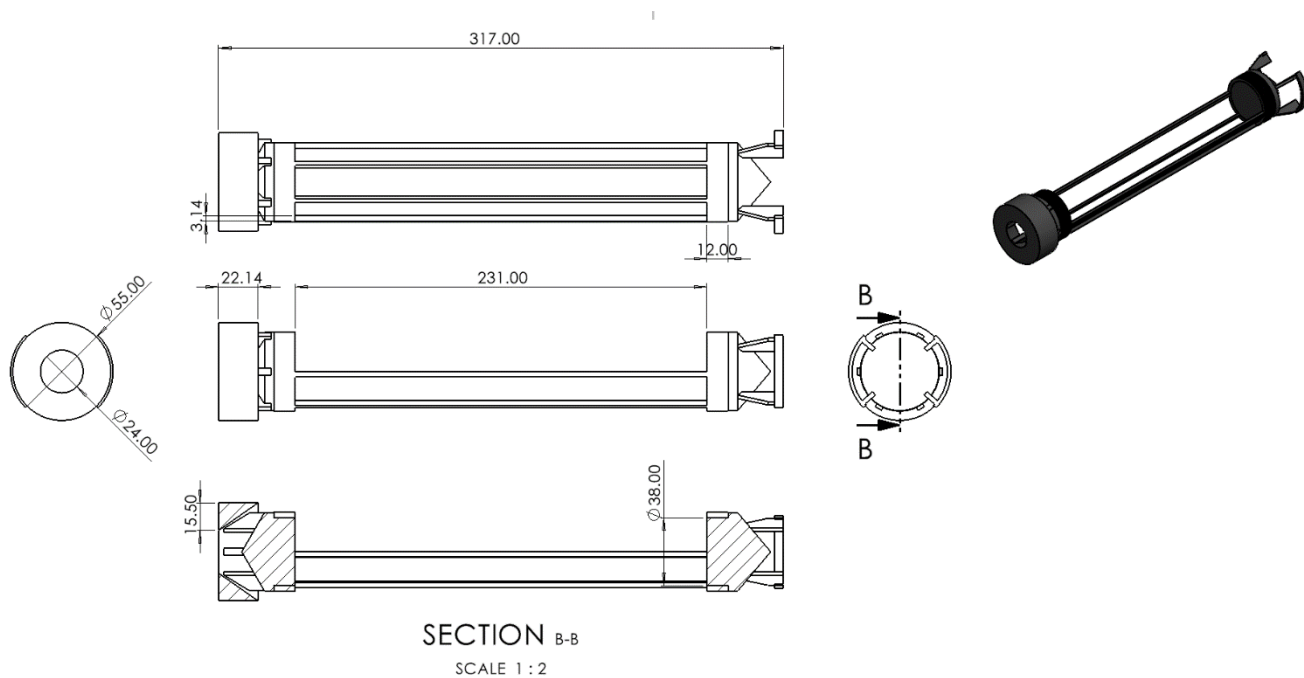
**Supplementary Fig.2.** 3D Drawings of the expanded device structures to show the assembly (and disassembly) of the MOF cartridge with the MOF housing and condenser components, between the night and day AWH cycles.



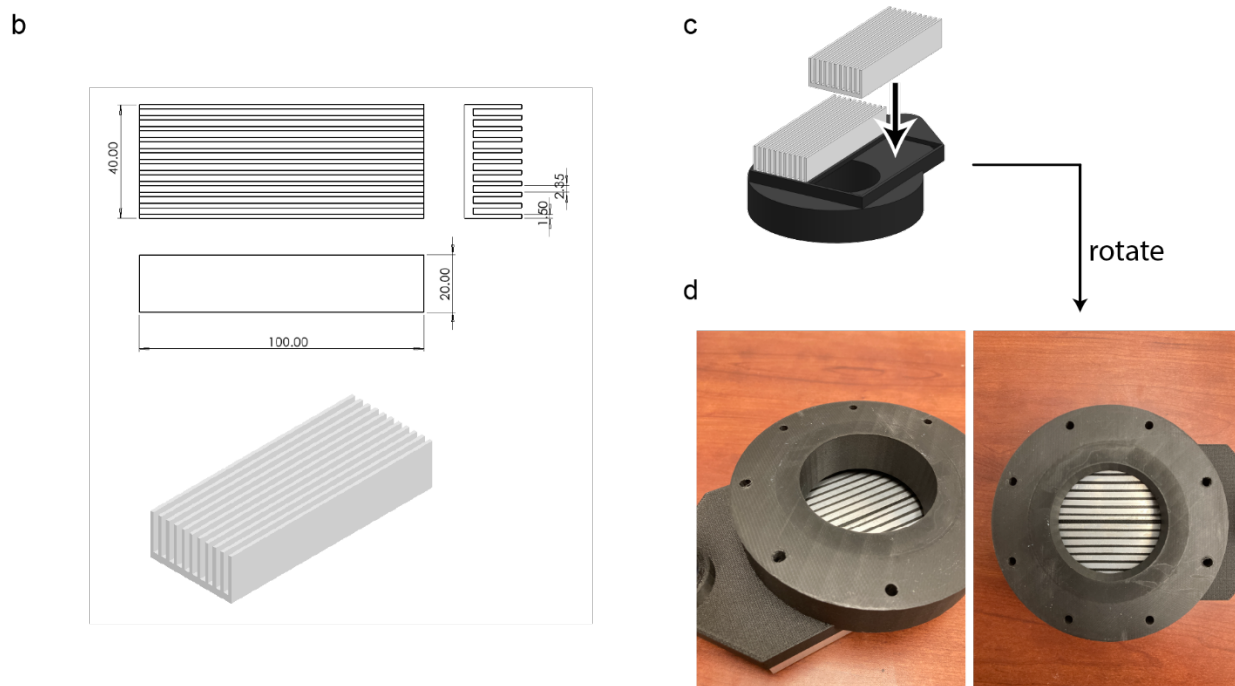
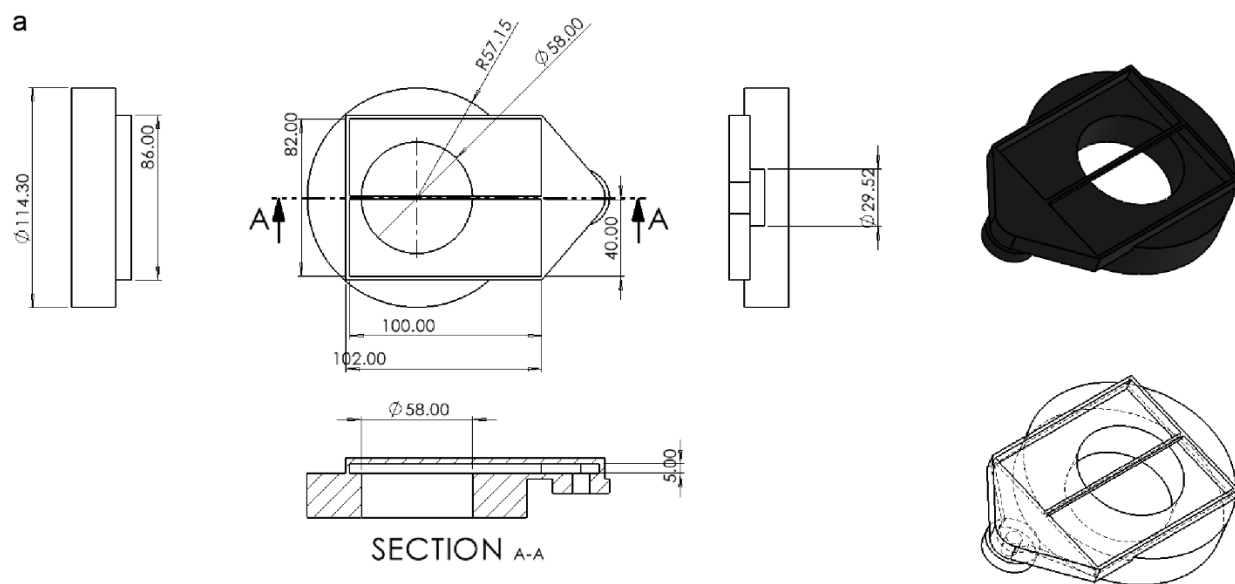
**Supplementary Fig.3.** Sectional view of the device to illustrate the direction of vapor and liquid water transport during the day cycles of AWH. Sectioned planes are capped with turquoise color for visual clarity.



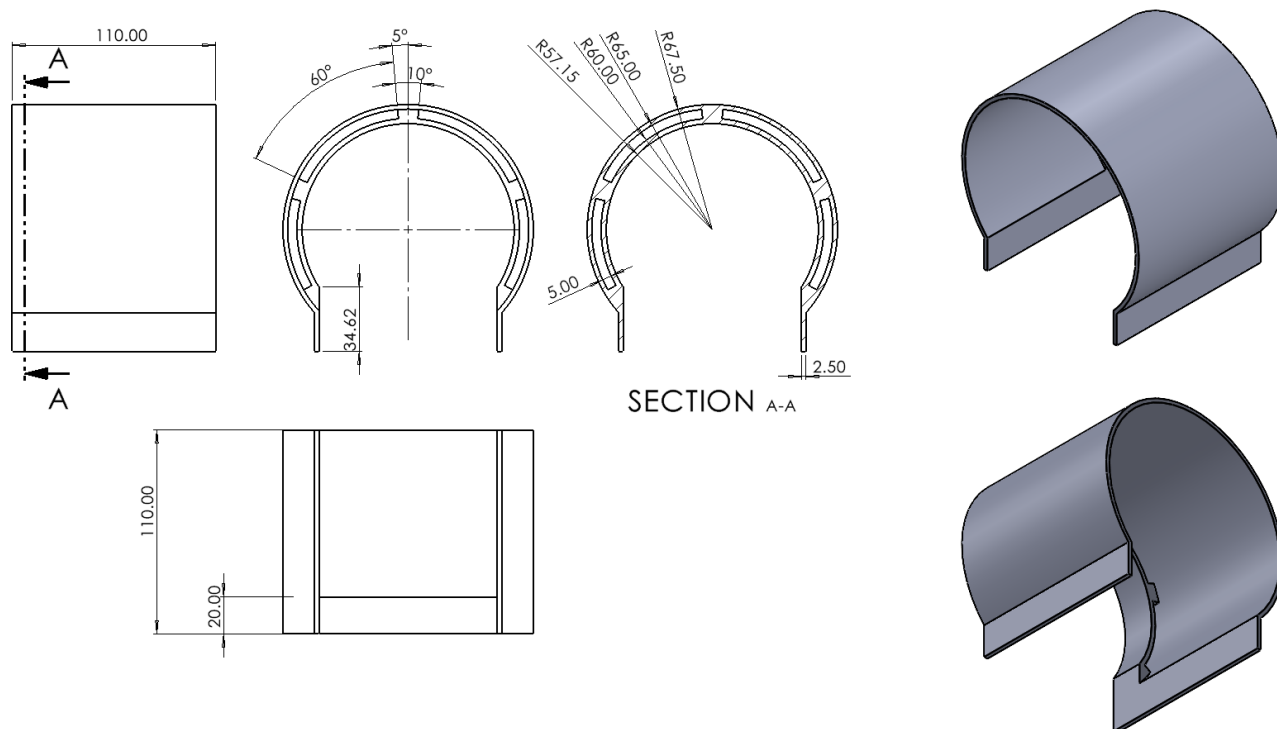
**Supplementary Fig.4.** (a) Drawings of the MOF housing part with the dimensions. The unit is millimeter (mm). (b) Photographs of the MOF housing part, showing the 1/8 FNPT threaded vacuum port and the valve connected to the outer shell of the housing. Vacuum port is not shown in the drawing models.



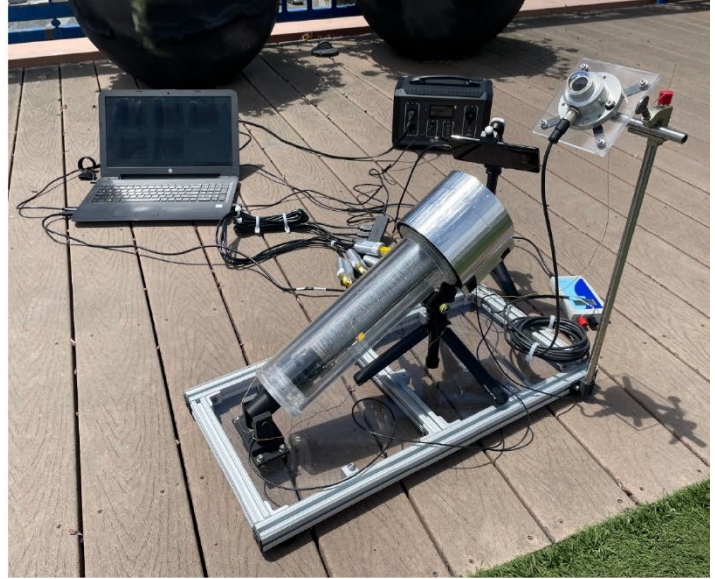
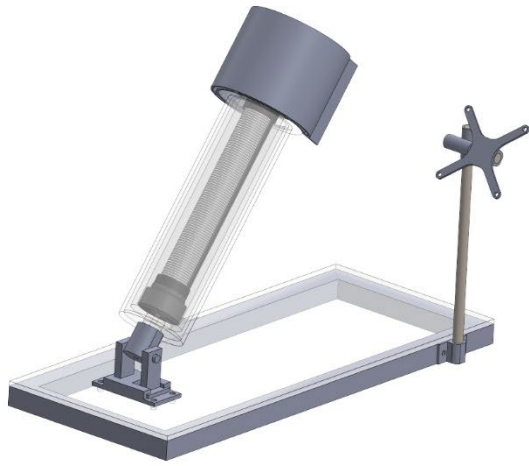
**Supplementary Fig.5.** Drawings of the MOF cartridge with the dimensions. The unit is millimeter (mm).



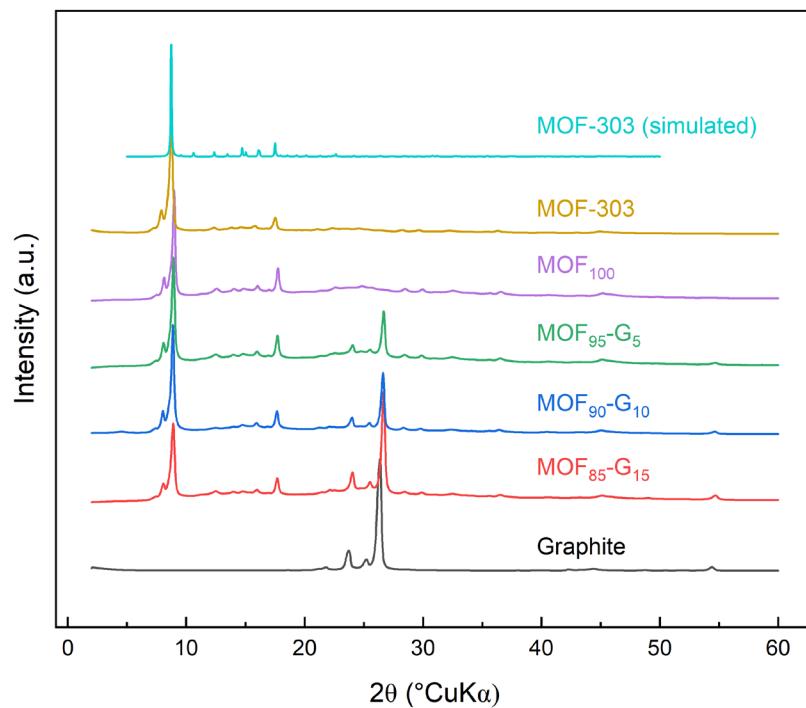
**Supplementary Fig.6.** Drawings of the (a) condenser housing and (b) aluminum heat sink parts with the dimensions. The unit is millimeter (mm). (c) Schematic illustration of assembling condenser housing and two heat sinks. Epoxy glue was applied to make leak-tight seals between the parts. (d) Photographs of the condenser part showing the CNF/PTFE patterned coating on condensation surface.



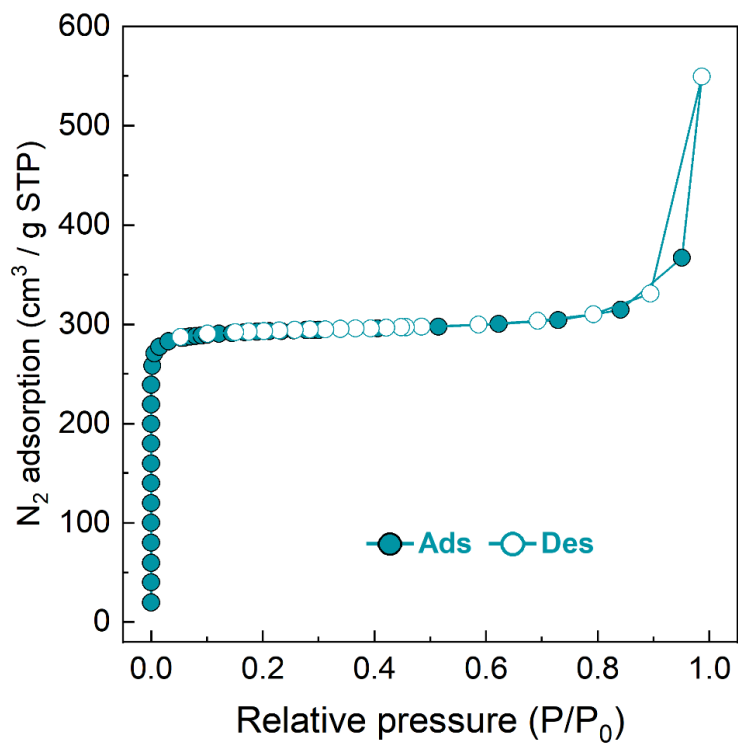
**Supplementary Fig.7.** Drawings of the light reflector part the dimensions. The unit is millimeters (mm).



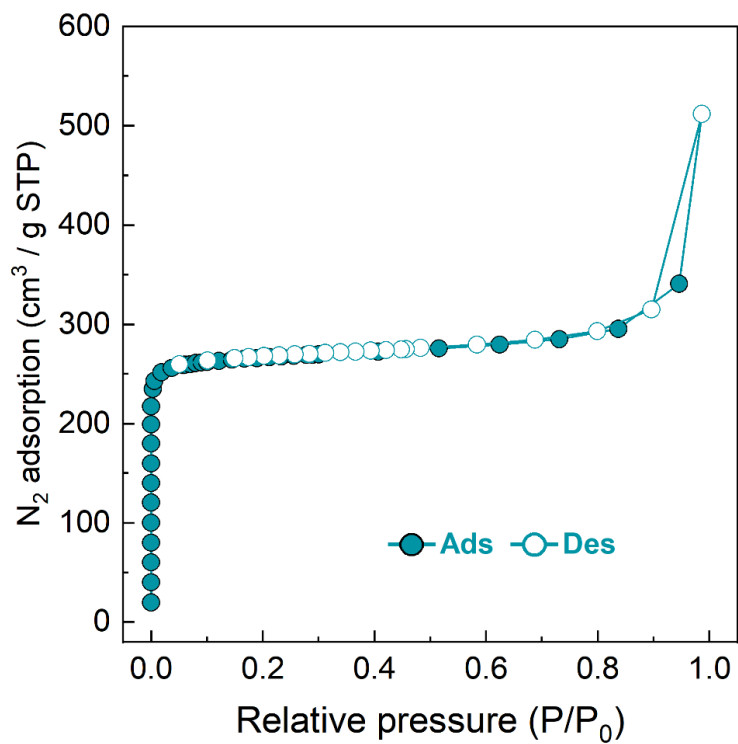
**Supplementary Fig.8.** Side-by-side comparison of the device modeling (left panel) and the entire device set-up including the measurement devices (right panel).



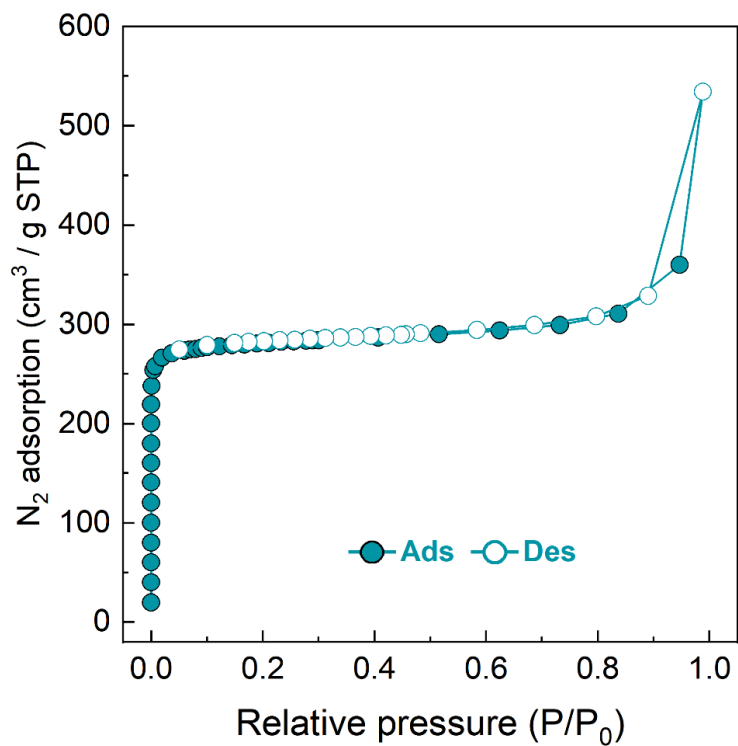
**Supplementary Fig.9.** PXRD spectra of MOF-303 simulated, activated MOF-303 and graphite powder, sorbent pellets prepared using MOF-303 without graphite (MOF<sub>100</sub>), 95 wt% MOF-303 and 5 wt% graphite (MOF<sub>95</sub>-G<sub>5</sub>), 90 wt% MOF-303 and 10 wt% graphite (MOF<sub>90</sub>-G<sub>10</sub>), and 85 wt% MOF-303 and 15 wt% graphite (MOF<sub>85</sub>-G<sub>15</sub>), respectively.



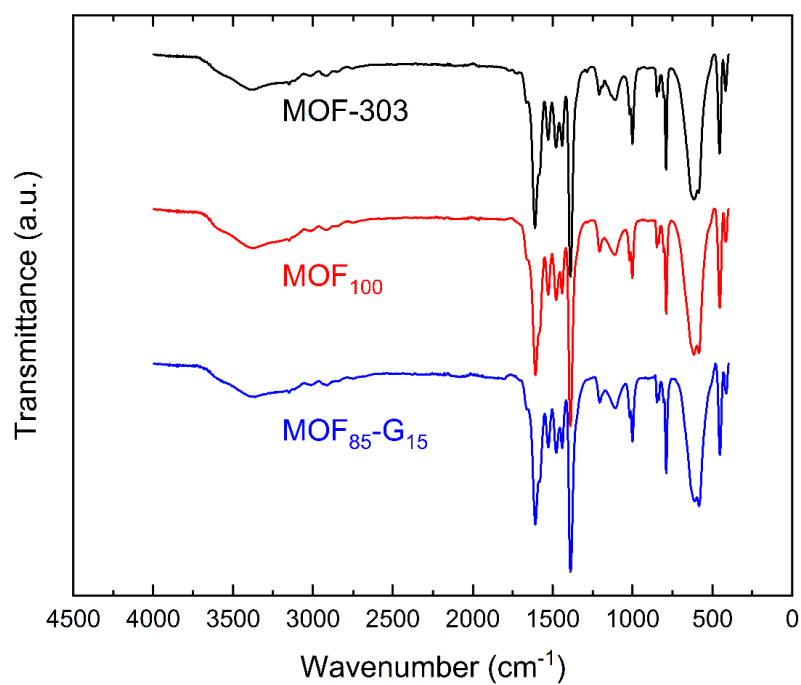
**Supplementary Fig.10.** N<sub>2</sub> isotherm (at 77 K) of the sorbent pellets prepared using MOF-303 without graphite binders. BET surface area is 1200 m<sup>2</sup>/g.



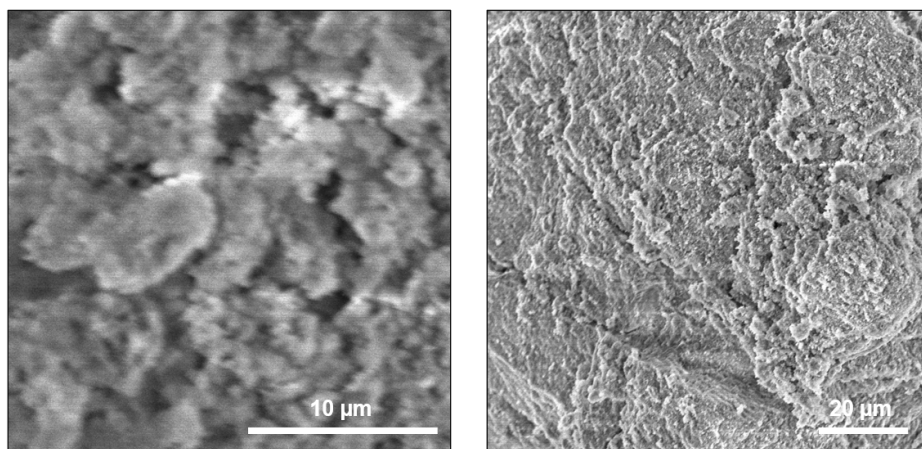
**Supplementary Fig.11.**  $N_2$  isotherm (at 77 K) of the sorbent pellets prepared using 95 wt% MOF-303 and 5 wt% graphite binders. BET surface area is 1080  $m^2/g$  pellet (1130  $m^2/g$  MOF-303).



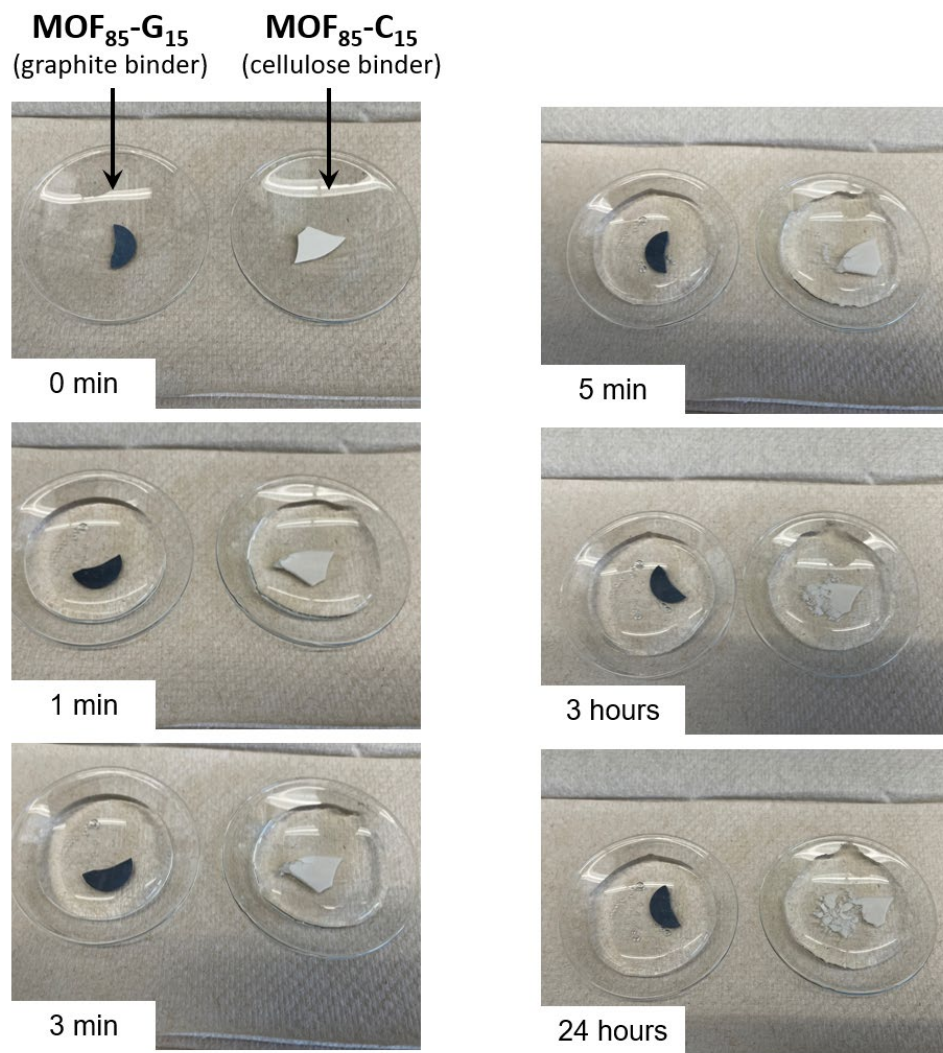
**Supplementary Fig.12.**  $N_2$  isotherm (at 77 K) of the sorbent pellets prepared using 90 wt% MOF-303 and 10 wt% graphite binders. BET surface area is  $1130 \text{ m}^2/\text{g}$  ( $1255 \text{ m}^2/\text{g}$  MOF-303).



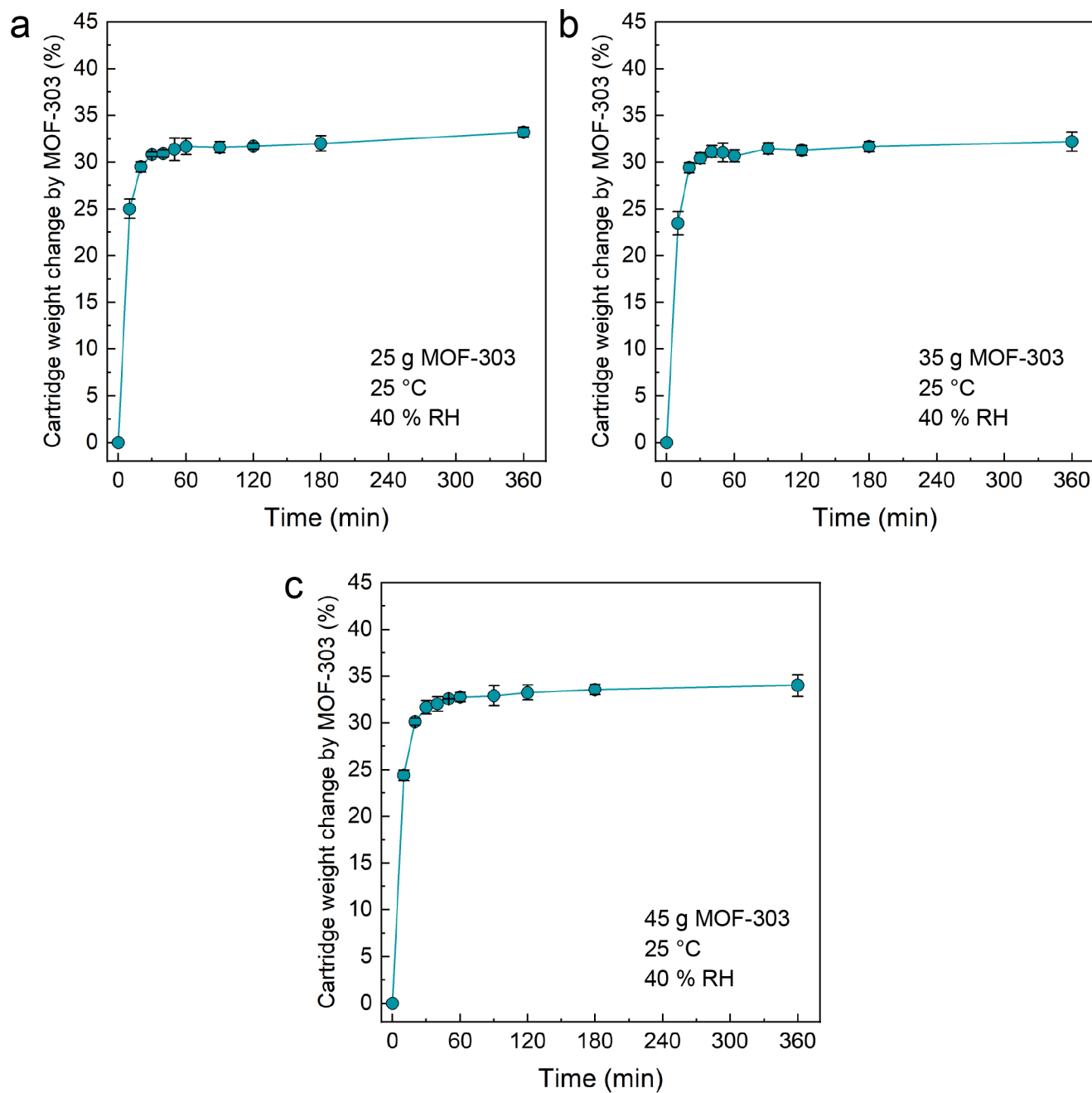
**Supplementary Fig.13.** FT-IR spectra of activated MOF-303 powder, sorbent pellets prepared using MOF-303 without graphite (MOF<sub>100</sub>) and 85 wt% MOF-303 and 15 wt% graphite binders (MOF<sub>85</sub>-G<sub>15</sub>), respectively.



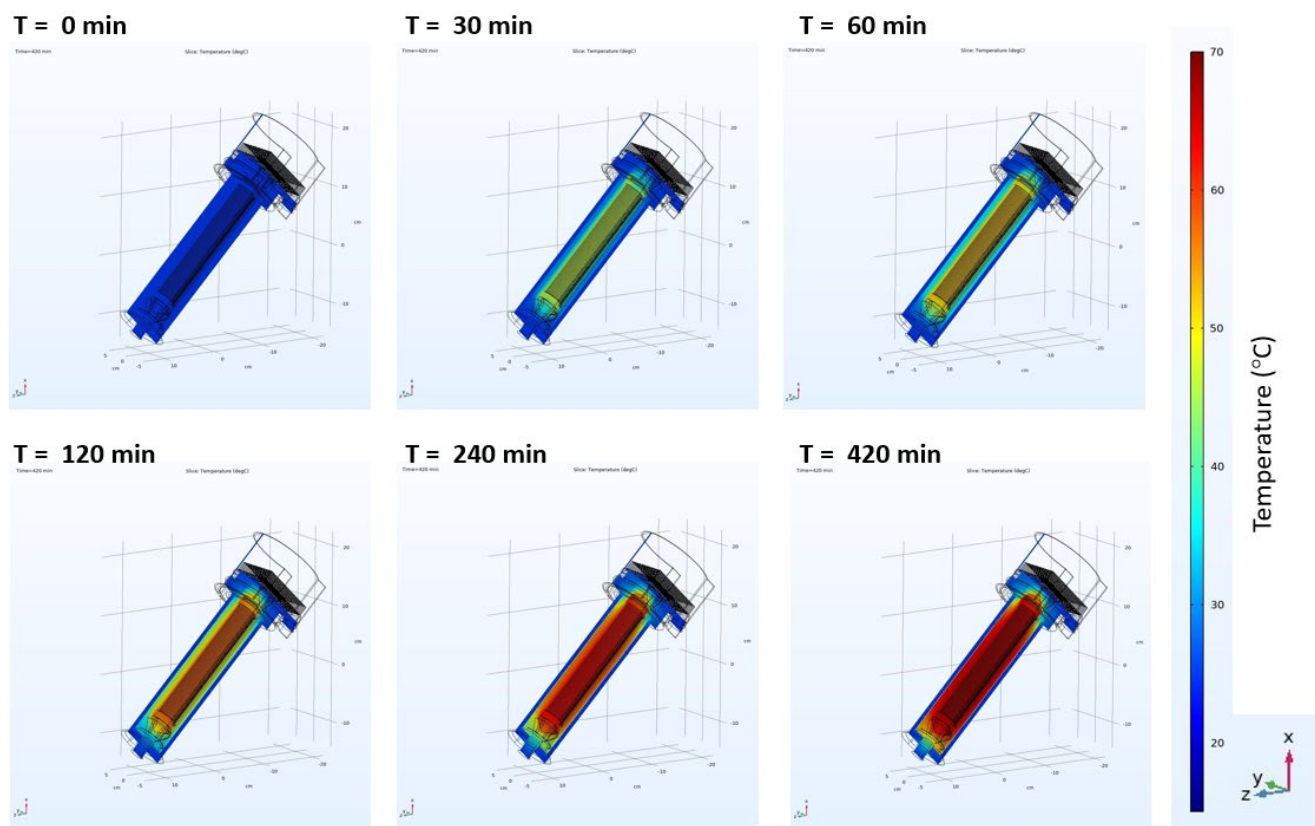
**Supplementary Fig.14.** SEM images of MOF<sub>85</sub>-G<sub>15</sub> pellet.



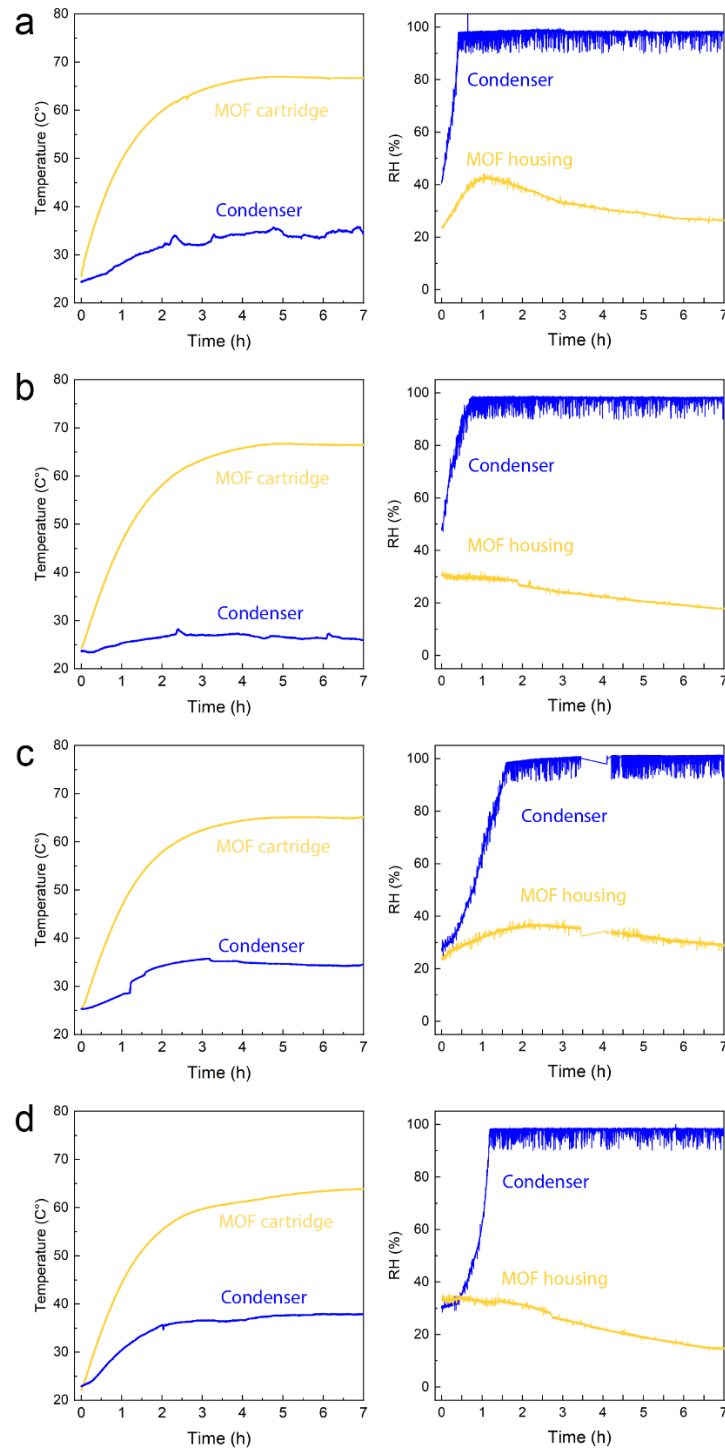
**Supplementary Fig.15.** Photographs of the fractured sorbent pellet pieces in water for 24 hours. The sorbent pellets were prepared using 85 wt% MOF-303 and 15 wt% graphite binders (MOF<sub>85</sub>-G<sub>15</sub>), and 85 wt% MOF-303 and 15 wt% cellulose binders (MOF<sub>85</sub>-C<sub>15</sub>), respectively.



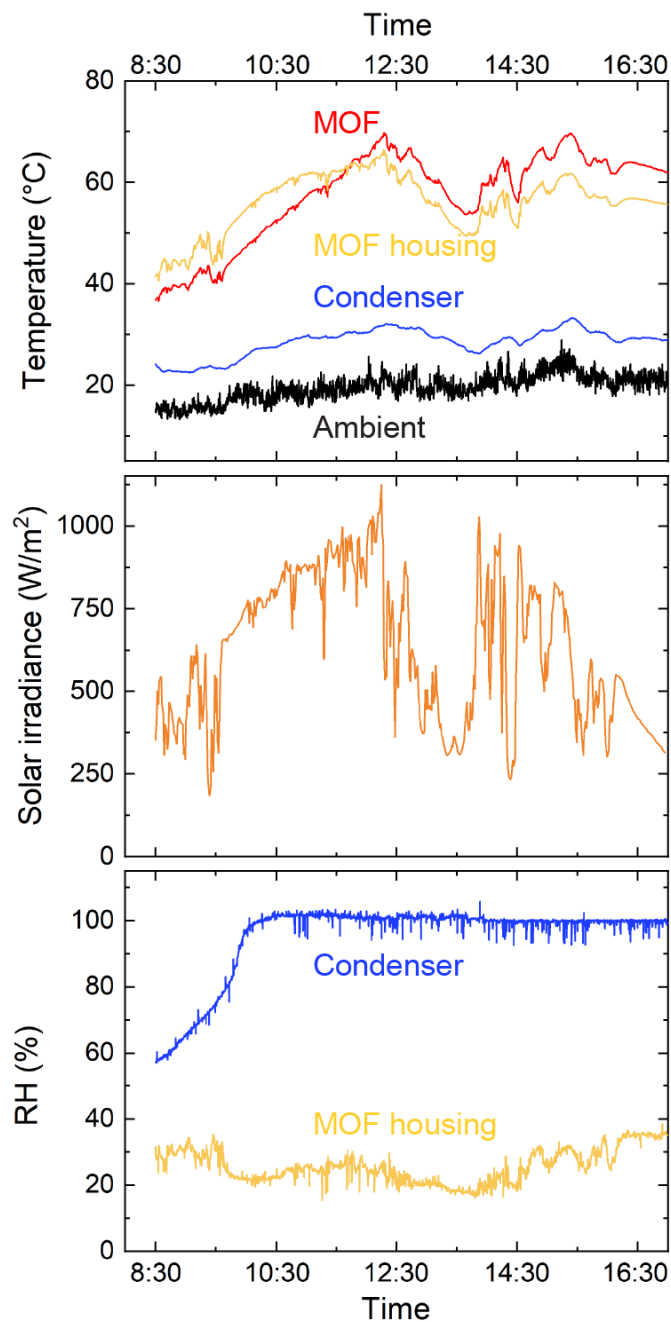
**Supplementary Fig.16.** Water uptake of MOF cartridge. Time-dependent weight change of the MOF cartridge at 25 °C and 40 % RH with the MOF-303 amounts of (a) 25 g, (b) 35 g and (c) 45 g, respectively. Error bars are the standard deviation of three independent measurements. Data are presented as mean values  $\pm$  SD ( $n = 3$ ).



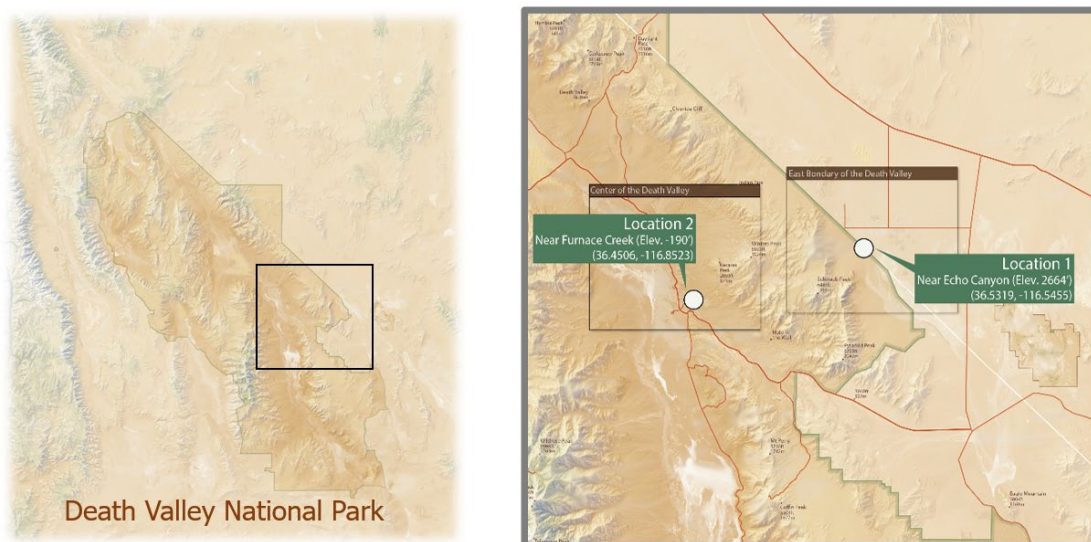
**Supplementary Fig.17.** Energy and heat transfer simulation of the device under the solar irradiance. (a) Time-dependent temperature plots of the device simulated for 7 hours (420 min). The direction of the external irradiation was set as  $(-1, 0, -1)$  during the course of simulation.



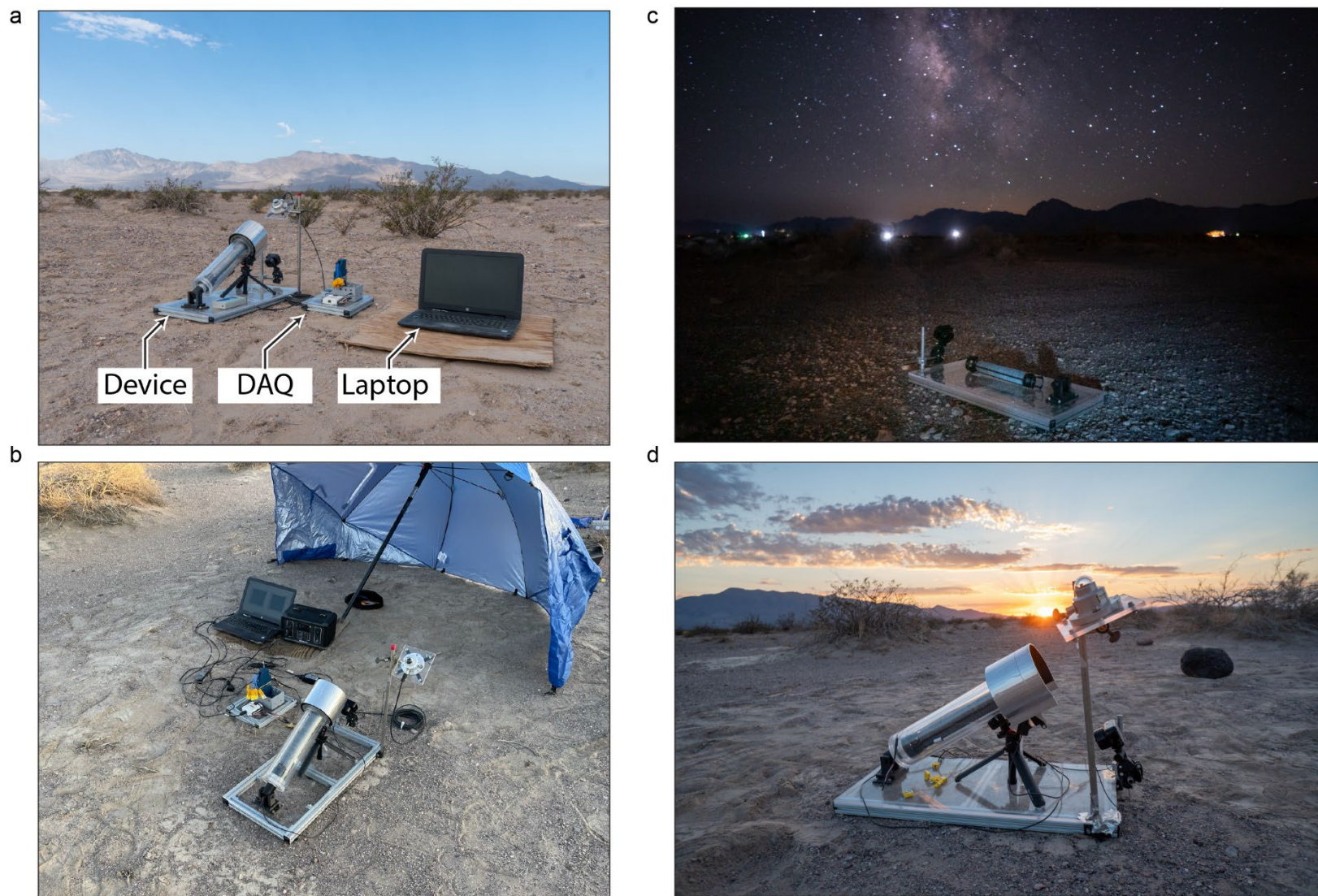
**Supplementary Fig.18.** Lab tests of the device using different condensers. Representative plots of temperature (°C, left panel) and RH (% , right panel) changes of the device using the condensers with (a) non-, (b) PTFE-, (c) CNF/PTFE-, and (d) pattern-coated surfaces.



**Supplementary Fig.19.** Temperature (°C), solar irradiance (W/m<sup>2</sup>), and RH (%) changes of the device and ambient air conditions during the Jun-2 test in Berkeley. Time axes are synced with each other.



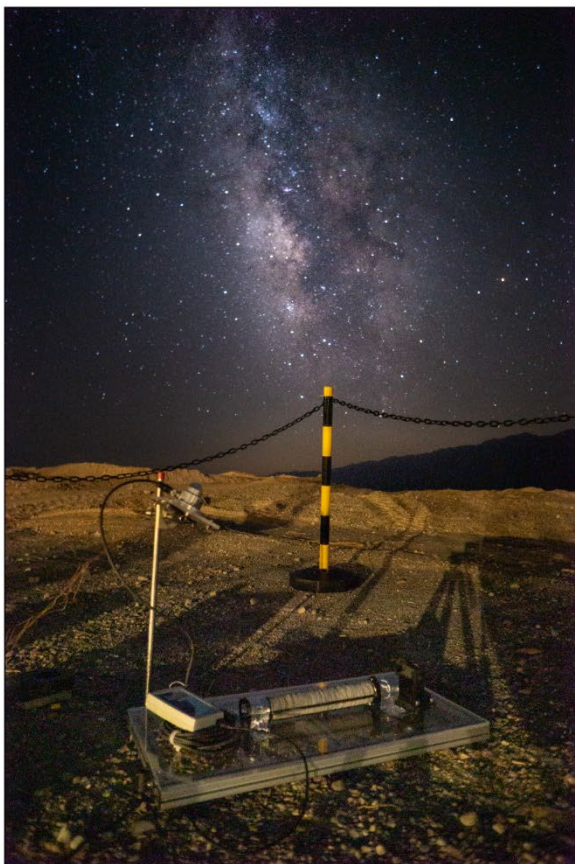
**Supplementary Fig. 20.** Locations of AWH in the Death Valley area. The tests were performed on the Location 1 (East boundary of the Death Valley, 36.5319° N, -116.5455° W) from August 19 2022 to August 21 2022, and on the Location 2 (Furnace Creek, 36.4506 ° N, -116.8523° W) from August 22 2022 to August 23 2022. These maps were from Harpers Ferry Center National Park Service (<https://www.nps.gov/subjects/hfc/index.htm>). OpenStreetMap®, licensed under the Open Data Commons Open Database License (ODbL).



**Supplementary Fig. 21.** Photographs of the device test in the Death Valley area ( $36.5319^{\circ}$  N,  $-116.5455^{\circ}$  W). (a) Device, data acquisition system (DAQ), and laptop without cable connection. (b) Photograph taken during the day cycle of the August 20 test with cable connections. Parasol was used to protect the electrical devices from the direct exposure to sunlight. (c) MOF cartridge during the night

cycle. (d) Device after the day cycle test is completed.

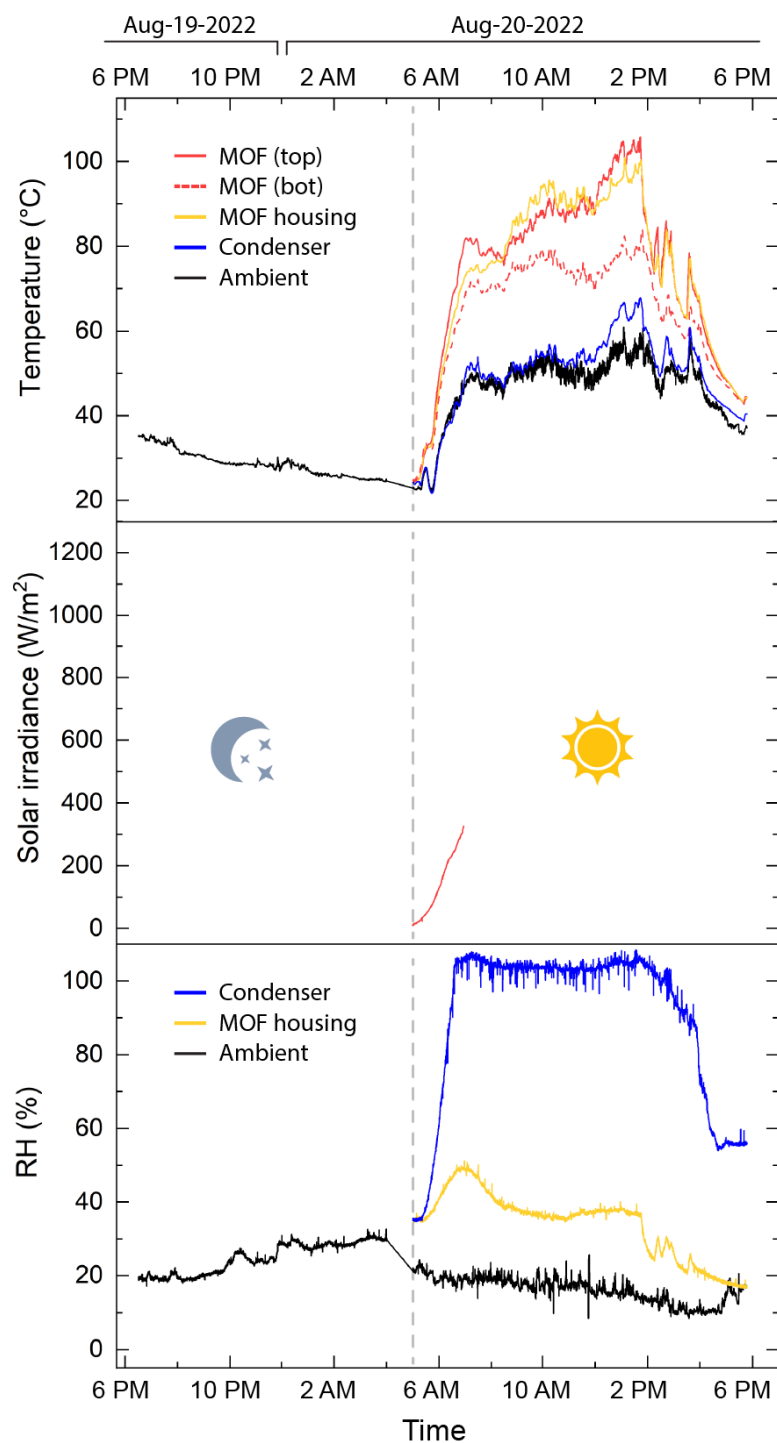
a



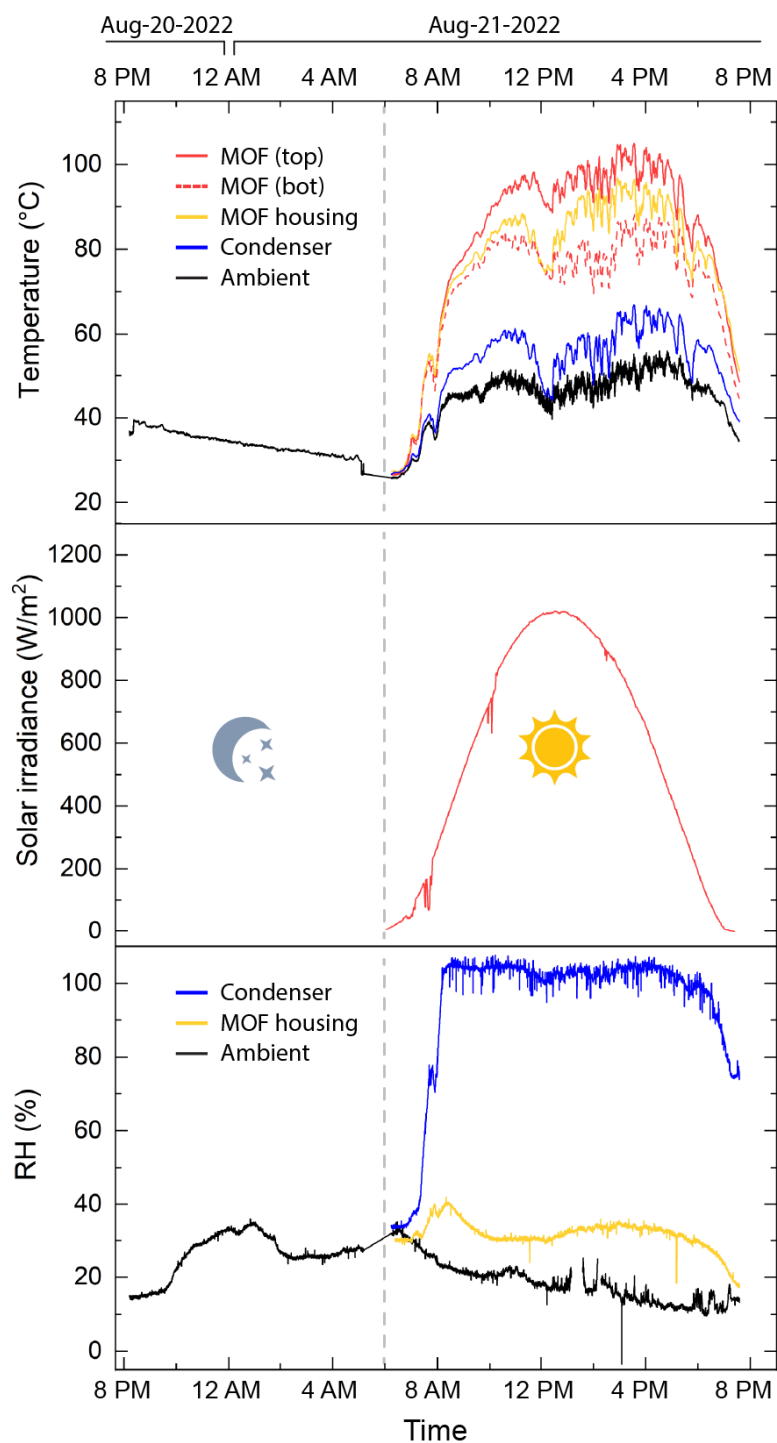
b



**Supplementary Fig. 22.** Photographs of the device test in the Furnace Creek ( $36.4506^{\circ}$  N,  $-116.8523^{\circ}$  W). (a) MOF cartridge during the night cycle of the August 23 2022 test. (b) Device at the end of the day cycle (after sun set). Red cargo box was used to protect the electrical devices from the direct exposure to sunlight.



**Supplementary Fig.23.** Temperature (°C), solar irradiance (W/m<sup>2</sup>), and RH (%) changes of the device and ambient air conditions during the August 20 test. Time axes are synced with each other. Recording of solar irradiance data was terminated at ~7 AM due to the malfunction of the measurement device.



**Supplementary Fig.24.** Temperature ( $^{\circ}\text{C}$ ), solar irradiance ( $\text{W}/\text{m}^2$ ), and RH (%) changes of the device and ambient air conditions during the August 21 test. Time axes are synced with each other.

**Supplementary Table 1.** Mass of water sorbed, desorbed, and harvested by the passive device.<sup>a</sup>

|                                          | Water sorption |              | Water desorption |              | Water harvested |              |
|------------------------------------------|----------------|--------------|------------------|--------------|-----------------|--------------|
|                                          | Weight (g)     | wt% by MOF   | Weight (g)       | wt% by MOF   | Weight (g)      | wt% by MOF   |
| Lab - Al <sup>b</sup>                    | 13.91 ± 0.04   | 39.76 ± 0.11 | 5.96 ± 0.82      | 17.04 ± 0.80 | 5.52 ± 0.27     | 15.76 ± 0.78 |
| Lab – PTFE <sup>b</sup>                  | 13.77 ± 0.04   | 39.35 ± 0.10 | 8.22 ± 0.58      | 23.47 ± 1.66 | 7.77 ± 0.58     | 22.19 ± 1.67 |
| Lab – CNF/PTFE <sup>b</sup>              | 13.79 ± 0.03   | 39.40 ± 0.10 | 7.76 ± 0.20      | 22.15 ± 0.58 | 7.31 ± 0.17     | 20.87 ± 0.48 |
| Lab - Patterned <sup>b</sup>             | 13.80 ± 0.05   | 39.43 ± 0.15 | 9.12 ± 0.25      | 26.04 ± 0.72 | 8.71 ± 0.25     | 24.89 ± 0.72 |
| Berkeley<br>(June 1)                     | 14.52          | 41.49        | 11.23            | 32.1         | 10              | 35.8         |
| Berkeley<br>(June 9)                     | 14.27          | 40.76        | 8.185            | 23.4         | 7.5             | 26.8         |
| Death Valley <sup>c</sup><br>(August 19) | ~11            | ~31.4        | ~9               | ~25.7        | 7.24            | 20.7         |
| Death Valley <sup>c</sup><br>(August 20) | ~10            | ~28.6        | ~8               | ~22.9        | 7.4             | 21.1         |
| Death Valley <sup>c</sup><br>(August 22) | ~6             | ~17.1        | ~4               | ~11.4        | 4.0             | 11.4         |

<sup>a</sup>Amount of MOF-303 for this table was 35 g.

<sup>b</sup>Lab test water sorption cycles were performed under 20 °C and 35% air condition inside the environmental chamber for 8 hours.

<sup>c</sup>Water sorption and desorption were measured by weighing MOF cartridge using a portable scale that has a precision of one gram.

**Supplementary Table 2.** Summary of the device field tests in Berkeley and the Death Valley areas.

|              | Date <sup>a</sup> | Night cycle |         | Day cycle |         | RH (%) during the night |      |                 | T (°C) during the day |      |      | I (W/m <sup>2</sup> ) |      |                                         | Water harvested (g) | AWH capacity (g·H <sub>2</sub> O/kg·MOF-303) |                       |
|--------------|-------------------|-------------|---------|-----------|---------|-------------------------|------|-----------------|-----------------------|------|------|-----------------------|------|-----------------------------------------|---------------------|----------------------------------------------|-----------------------|
|              |                   | Start       | End     | Start     | End     | High                    | Low  | Avg.            | High                  | Low  | Avg. | High                  | Avg. | Total <sup>d</sup> (MJ/m <sup>2</sup> ) |                     | per day                                      | per hour <sup>c</sup> |
| Berkeley     | Jun 1~2           | -           | -       | 8:30 AM   | 4:30 PM | -                       | -    | 86 <sup>b</sup> | 28.9                  | 13.2 | 19.6 | 1125                  | 620  | 19                                      | ~10                 | ~285                                         | ~35.8                 |
|              | Jun 9~10          | -           | -       | 8:30 AM   | 4:30 PM | -                       | -    | 62 <sup>b</sup> | 38.2                  | 23.7 | 31.5 | 1020                  | 770  | 23.7                                    | ~7.5                | ~214                                         | ~26.8                 |
| Death Valley | Aug 19~20         | 7:45 PM     | 5:15 AM | 6:30 AM   | 7:15 PM | 32.8                    | 17.2 | 24.8            | 60.1                  | 21.9 | 46.5 | -                     | -    | -                                       | ~7.24               | ~207                                         | ~16.2                 |
|              | Aug 20~21         | 8:15 PM     | 5:15 AM | 6:16 AM   | 7:30 PM | 35.9                    | 13.8 | 26.2            | 56.0                  | 25.6 | 45.0 | 1020                  | 570  | 27.3                                    | ~7.4                | ~210                                         | ~16.0                 |
|              | Aug 22~23         | 7:15 PM     | 5:15 AM | 6:30 AM   | 7:30 PM | 21.0                    | 9.4  | 14              | 60.7                  | 34.0 | 51.6 | 1025                  | 580  | 27.5                                    | ~4.0                | ~114                                         | ~8.8                  |

RH: relative humidity, T: temperature, I: solar irradiance intensity, AWH: atmospheric water harvesting, Avg.: average.

<sup>a</sup>Year is 2022.

<sup>b</sup>These RH values were obtained from publicly available Berkeley weather information.

<sup>c</sup>Hour-based AWH capacity was calculated by dividing the per-day capacity by the hours of each day cycles.

<sup>d</sup>Total solar irradiance during the day cycles.

## References

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