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Metal-Organic Framework-based Atmospheric Water Harvesting for Enhanced Photovoltaic Efficiency and Sustainability

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Experimental:

Materials

All reagents including the organic ligand used in this study 3,3”,5,5”-tetrakis(4-carboxyphenyl)-p-terphenyl (H_4 TCPT) were obtained from commercial sources and used without further purification.

Synthesis of Cr-soc-MOF-1. Prior to the synthesis, a solution of $FeCl_3 \cdot 6H_2O$ was prepared in 50 mL N,N′ -dimethylformamide (DMF), with (900 mg, 3.3 mmol) was added to a 500 L pressure flask with a dissolved 3,3″ ,5,5″ -tetrakis(4-carboxyphenyl)-p-terphenyl (H_4TCPT) (1050 mg, 1.5 mmol) in DMF (25 mL), and acetonitrile (CH_3CN) (75 mL). Then a stock solution of nitric acid in DMF (3.5 M) was prepared, from that (105 mL) was added to the reaction mixture followed by sonication for 15 mins. The clear orange-yellow solution was

subsequently placed in a preheated oven at 115 °C for 48 h to give pure orange-yellow cubic shaped crystals. After synthesis, the crystals were washed to remove any extra metal salts with DMF until the color of the supernatant turned colorless. Then the crystals were soaked in 50 mL CH_3CN for one day. In preparation to exchange the sample with $CrCl_2$, the solvent was removed, and the material was charged in a 100 mL blue cap glass container under an inert atmosphere. Then a solution of 1500 mg of $CrCl_2$ dissolved in 20 mL DMF was added. The vial was then placed in a preheated oven with a fixed temperature of 115 °C for 18 h before removing it. The green product was washed with DMF several times until the supernatant turned colorless. (Yield 1 g).

MOF coating on heat sink fin: The Cr-**soc**-MOF was coated on the surface of the heat fins on a commercialized heat sink via spray coating. The MOF suspension (2.5 mg MOF/1 mL ethanol solvent) was loaded into a 100 ml plastic sprayer and the MOF–suspension solution and promptly sprayed onto the heat fins for 30 seconds in each cycle, followed by drying under ambient conditions for 2 minutes. The spraying and drying process was repeated until desired loading weight of the MOF was achieved (see Figure S1).

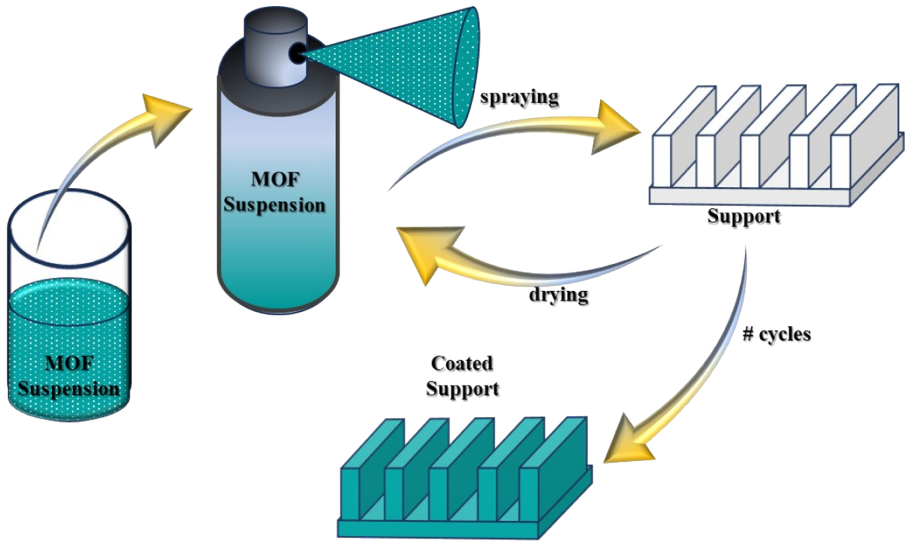

Figure S1. . Schematic of the MOF coating process on the commercial heat fins.

PV panel cooling test. The characteristics of the PV panel (i.e., the V_{oc}, Efficiency, and P_{max}) under different sunlight intensities were investigated on a Keithley-2400 source meter. The prototype device with a MOF-coated heatsink was first placed inside a humidity chamber with a temperature of ~22 °C and relative humidity of ~90% overnight to adsorb water vapor. The prototype was subsequently irradiated by the simulated sunlight generated from an Oriel

94023A solar simulator equipped with AM 1.5 filter. The temperature change of the PV panel was measured and recorded by an infrared camera (FLIR 655SC). The mass change of the coated MOF was measured and recorded using a computer-connected electronic scale.

The PV panel involved in this work was composed of nine PV cells connected in series and the total effective PV cell area was 18.2 cm^2. The sunlight intensity from the solar simulator was tuned to be 0.8, 0.9, 1.0, and 1.1 kW/m^2 to reflect the variation of the highest sunlight intensities during a summer day. Our previous research has demonstrated that the time required for a full water vapor adsorption of the sorbent was highly dependent on the thickness of the sorbent and the ambient humidity. Thereby, the coating thickness of MOF was desired to be 1-2 mm (the estimated thickness of MOF coating layer) and was placed in a high humidity condition to ensure a reasonable water vapor adsorption period. The dry weight of the coated MOF before water vapor adsorption was 1.1-1.2 g (dry weight of MOF) and the weight of the adsorbed water after the water vapor sorption process was ~1.3 g.

COMSOL model and simulation: A COMSOL Multiphysics model was constructed to simulate the cooling performance at practical condition. A model with a prototype dimension matched the lab test device was built to assure the accuracy of the simulation results. An enlarged model with the PV dimension of 1×2 m^2 with the compatible size of a MOF-coated heat sink was further established to predict the feasibility of the cooling principle in practical applications.

Powder X-ray Diffraction (PXRD) Patterns:

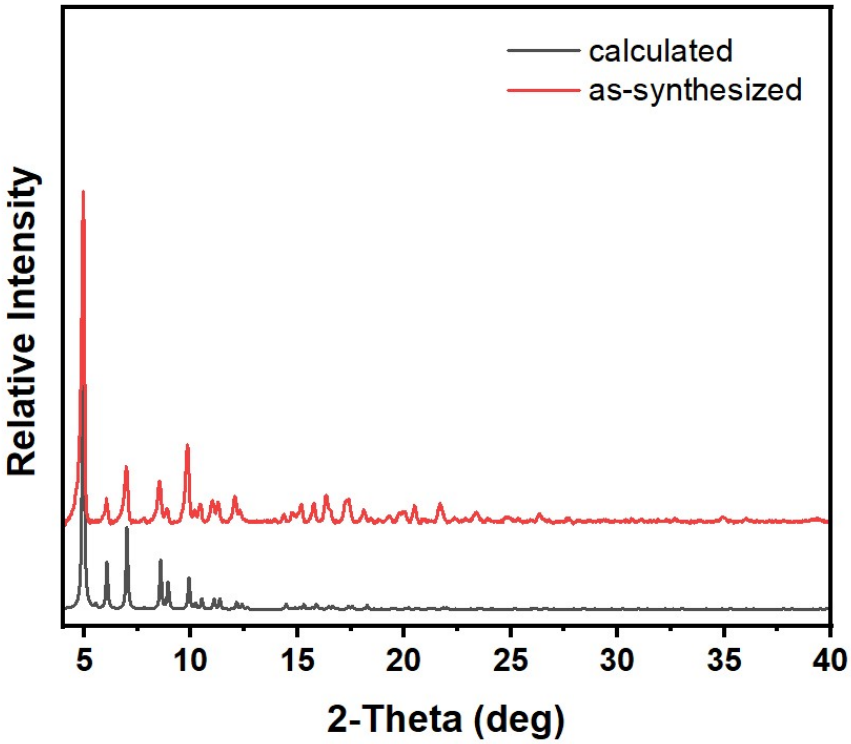

Figure S2. Experimental and calculated powder X-ray diffraction (PXRD) patterns for Cr-**soc**-MOF-1, indicating the purity of the as-synthesized material.

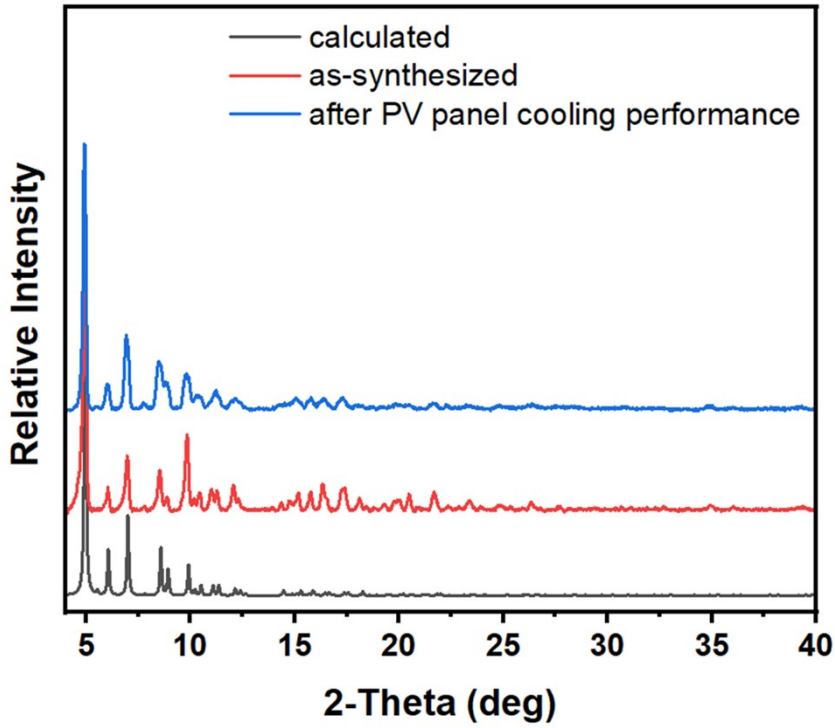

Figure S3. PXRD patterns for Cr-**soc**-MOF-1 after PV panel cooling performance, indicating the stability of the material after performing the test.

Table S1. Electricity Improvement Based Cooling Comparison of Generation Using AWH-Materials

Material	Percentage Increase in Electricity Generation	reference
Cr-**soc**-MOF-1	7.5%	This work
PAM-CNT-CaCl2	13–19%	1
Li-PAAm hydrogel	14.5% to 15.5%	2
silica gel	1.2%	3
MIL-160	3%	3
CAU-10	4%	3
Al-Fum	5.1%	3

References:

Li, R.; Shi, Y.; Wu, M.; Hong, S.; Wang, P., Photovoltaic Panel Cooling by Atmospheric Water Sorption–Evaporation Cycle. Nature Sustainability 2020, 3 (8), 636-643.

Pu, S.; Fu, J.; Liao, Y.; Ge, L.; Zhou, Y.; Zhang, S.; Zhao, S.; Liu, X.; Hu, X.; Liu, K.; Chen, J., Promoting Energy Efficiency Via a Self-Adaptive Evaporative Cooling Hydrogel. Advanced Materials 2020, 32 (17), 1907307.

Gkaniatsou, E.; Meng, B.; Cui, F.; Loonen, R.; Nouar, F.; Serre, C.; Hensen, J., Moisture-Participating Mof Thermal Battery for Heat Reallocation between Indoor Environment and Building-Integrated Photovoltaics. Nano Energy 2021, 87, 106224.