

Supplementary Materials

Efficient solar-driven interfacial steam-hydropower co-generation by high-quality carbon nanotube from discarded polyolefin separator

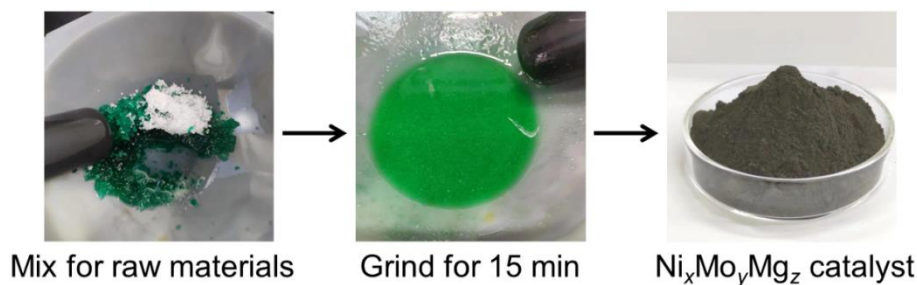
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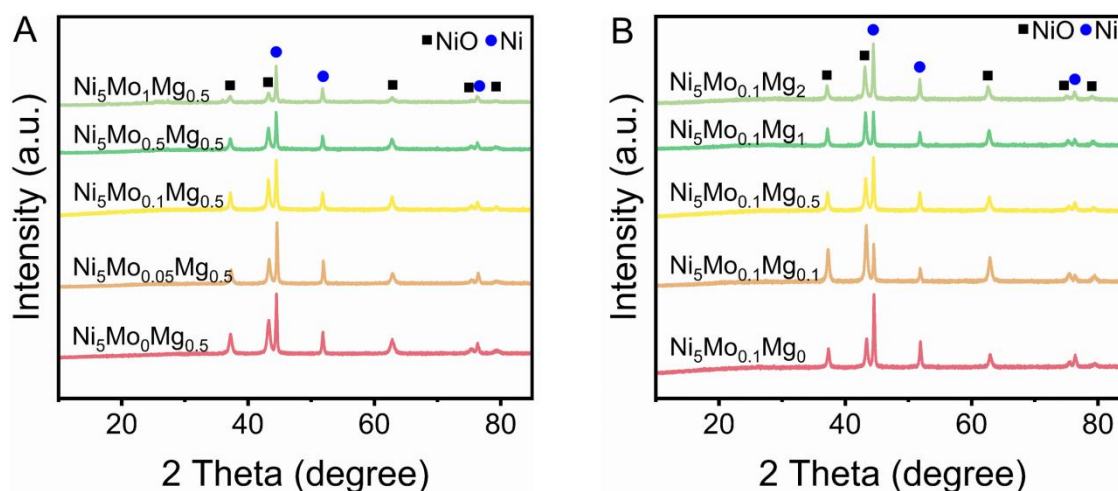
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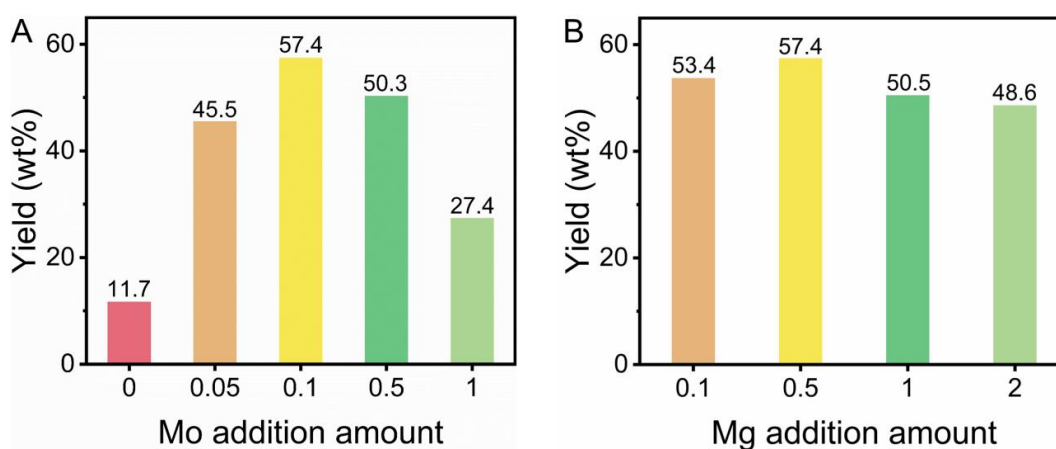
Supplementary Figure 1. Photographs of discarded PE separators.



Supplementary Figure 2. The preparation process of $\text{Ni}_x\text{Mo}_y\text{Mg}_z$ catalyst.

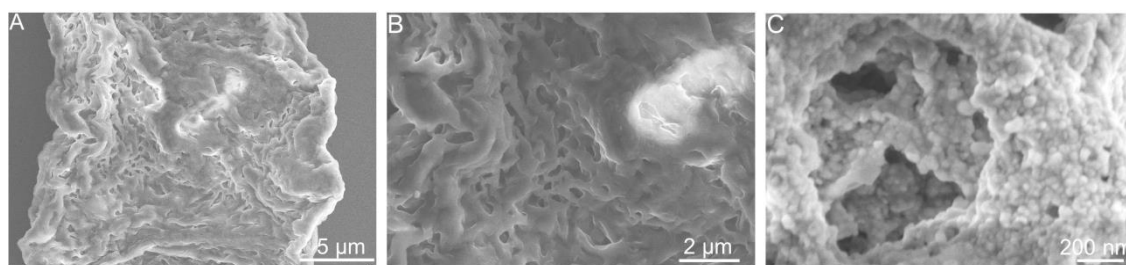


Supplementary Figure 3. XRD patterns of (A) $\text{Ni}_5\text{Mo}_y\text{Mg}_{0.5}$ and (B) $\text{Ni}_5\text{Mo}_{0.1}\text{Mg}_z$.

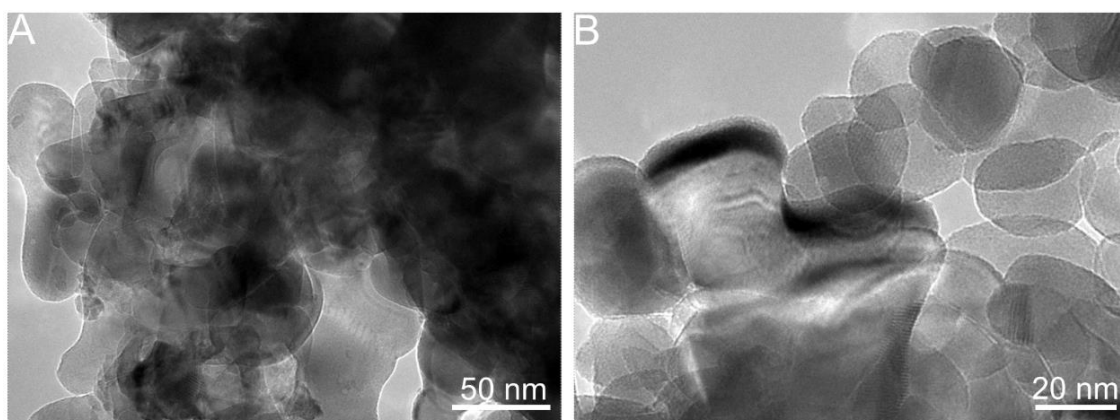


Supplementary Figure 4. The yield of CNT_{x-y-z} using (A) $\text{Ni}_5\text{Mo}_y\text{Mg}_{0.5}$ and (B) $\text{Ni}_5\text{Mo}_{0.1}\text{Mg}_z$.

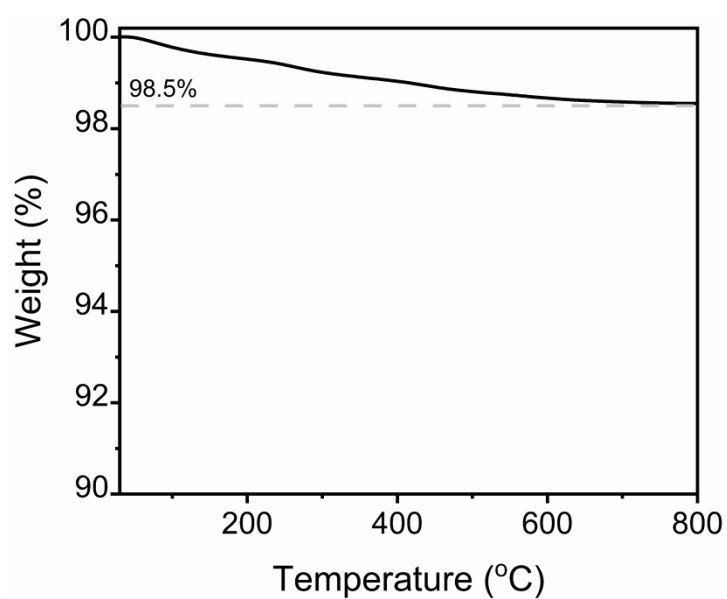
Note: When $\text{Ni}_5\text{Mo}_{0.1}\text{Mg}_0$ is used as the catalyst, the product is aggregated spherical carbon particles with the size of 50–200 nm, rather than CNTs. The yield of spherical carbon particles is calculated to be 16.5 wt%.



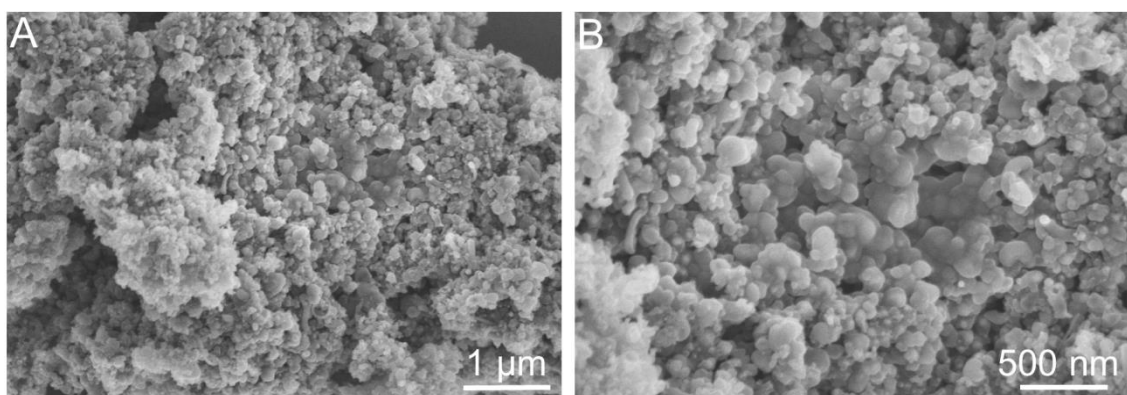
Supplementary Figure 5. (A-C) SEM images of $\text{Ni}_5\text{Mo}_{0.1}\text{Mg}_{0.5}$ catalyst.



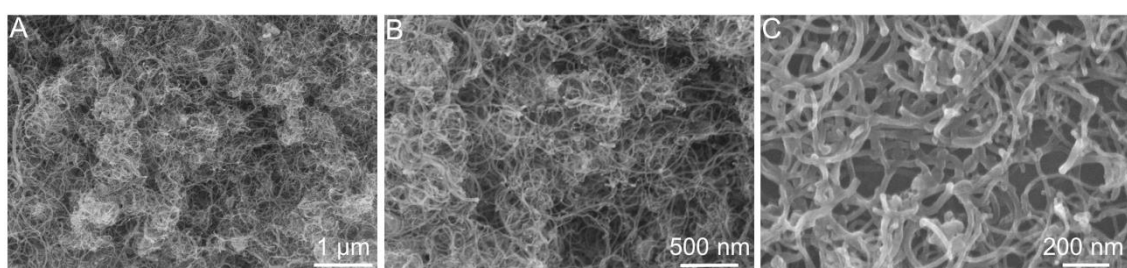
Supplementary Figure 6. (A and B) TEM images of $\text{Ni}_5\text{Mo}_{0.1}\text{Mg}_{0.5}$ catalyst.



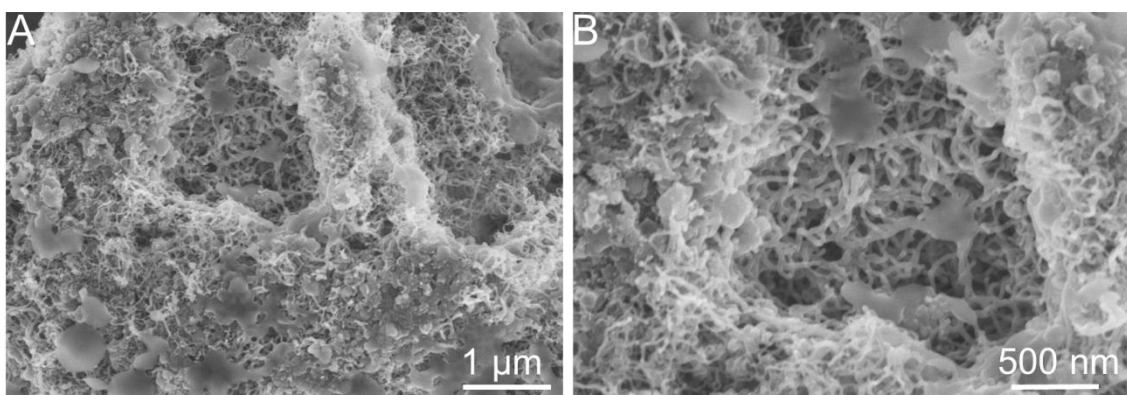
Supplementary Figure 7. TGA curve of $\text{Ni}_5\text{Mo}_{0.1}\text{Mg}_{0.5}$ catalyst.



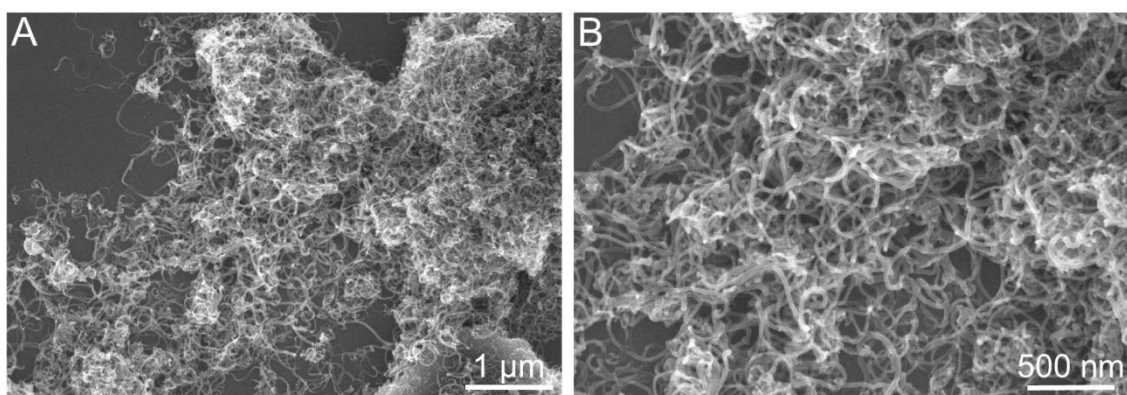
Supplementary Figure 8. (A and B) SEM images of OCNT_{5-0.1-0}.



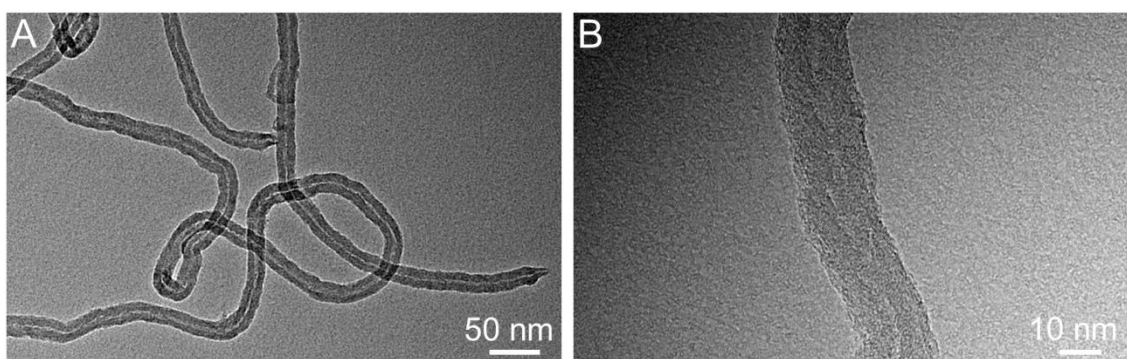
Supplementary Figure 9. (A-C) SEM images of OCNT_{5-0.1-2}.



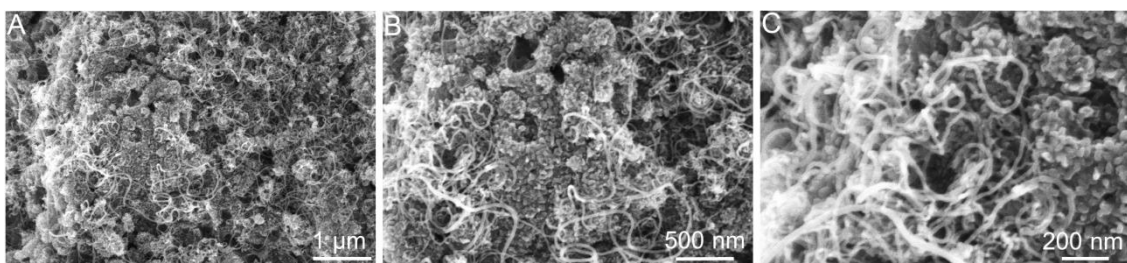
Supplementary Figure 10. (A and B) SEM images of OCNT_{5-0-0.5}.



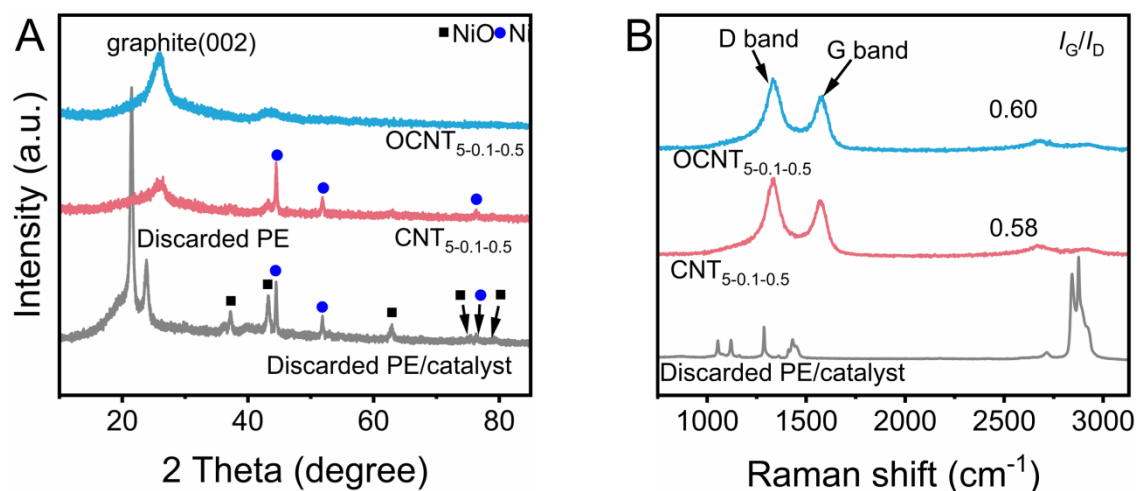
Supplementary Figure 11. (A and B) SEM images of OCNT_{5-0.1-0.5}.



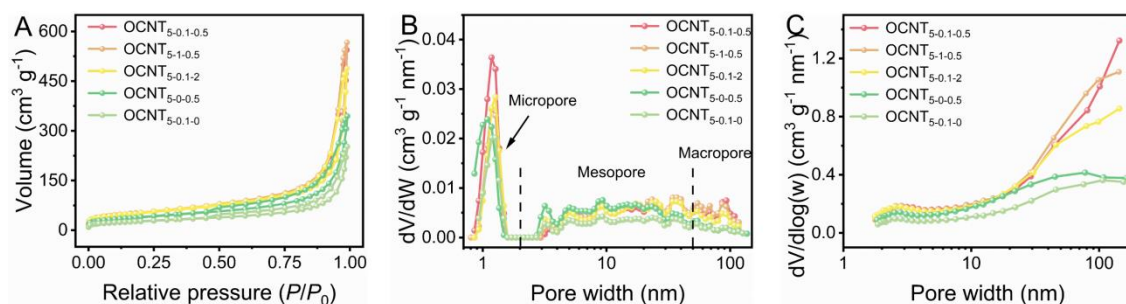
Supplementary Figure 12. (A and B) TEM images of OCNT_{5-0.1-0.5}.



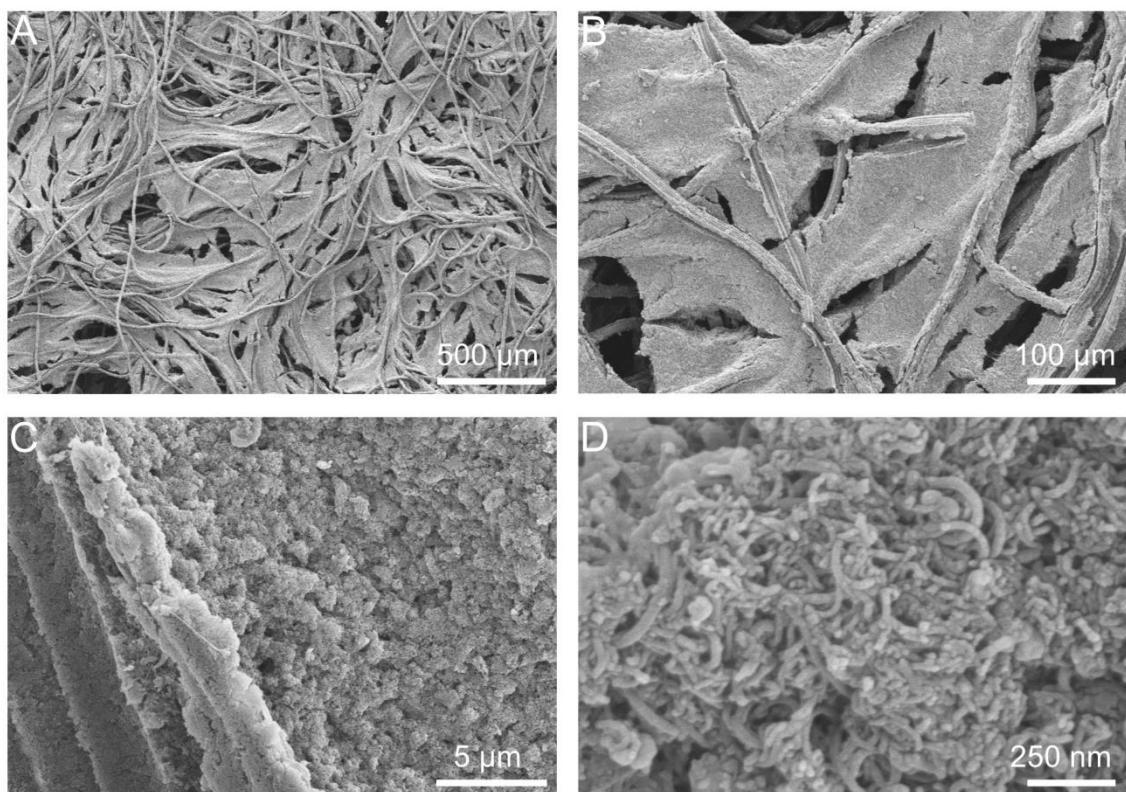
Supplementary Figure 13. (A-C) SEM images of OCNT_{5-1-0.5}.



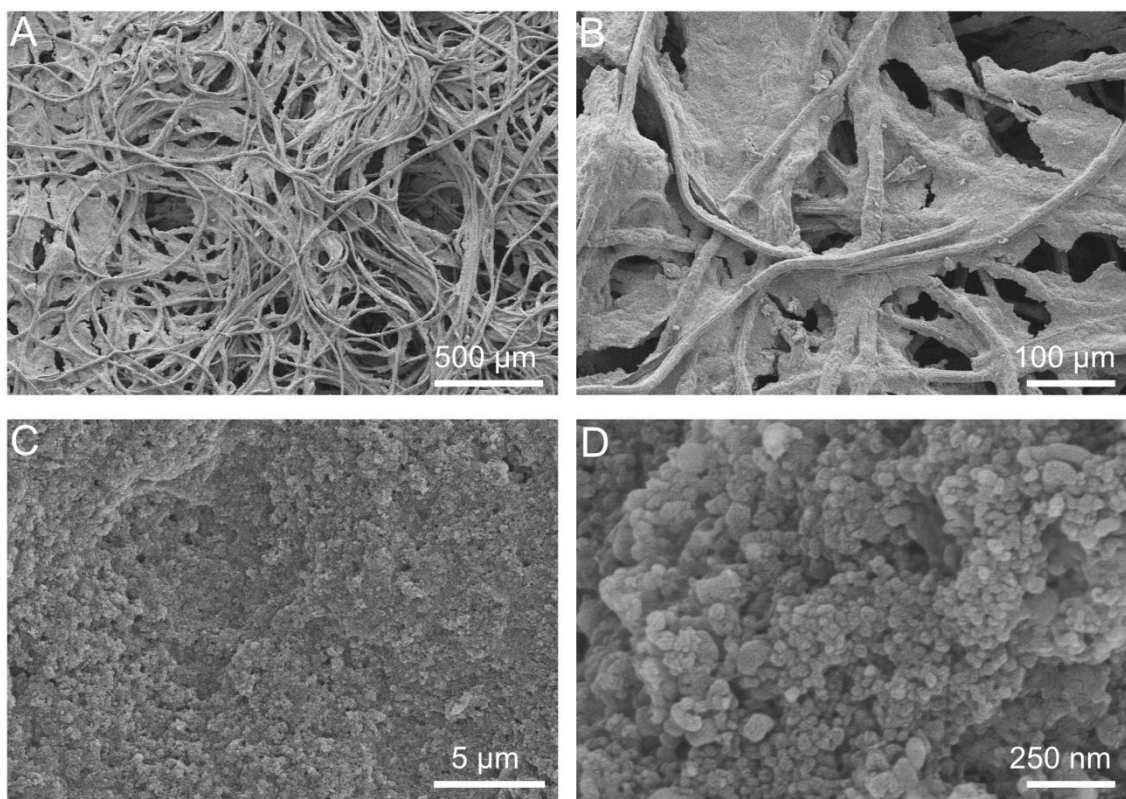
Supplementary Figure 14. (A) XRD patterns and (B) Raman spectra of OCNT_{5-0.1-0.5}, CNT_{5-0.1-0.5} and discarded PE/catalyst.



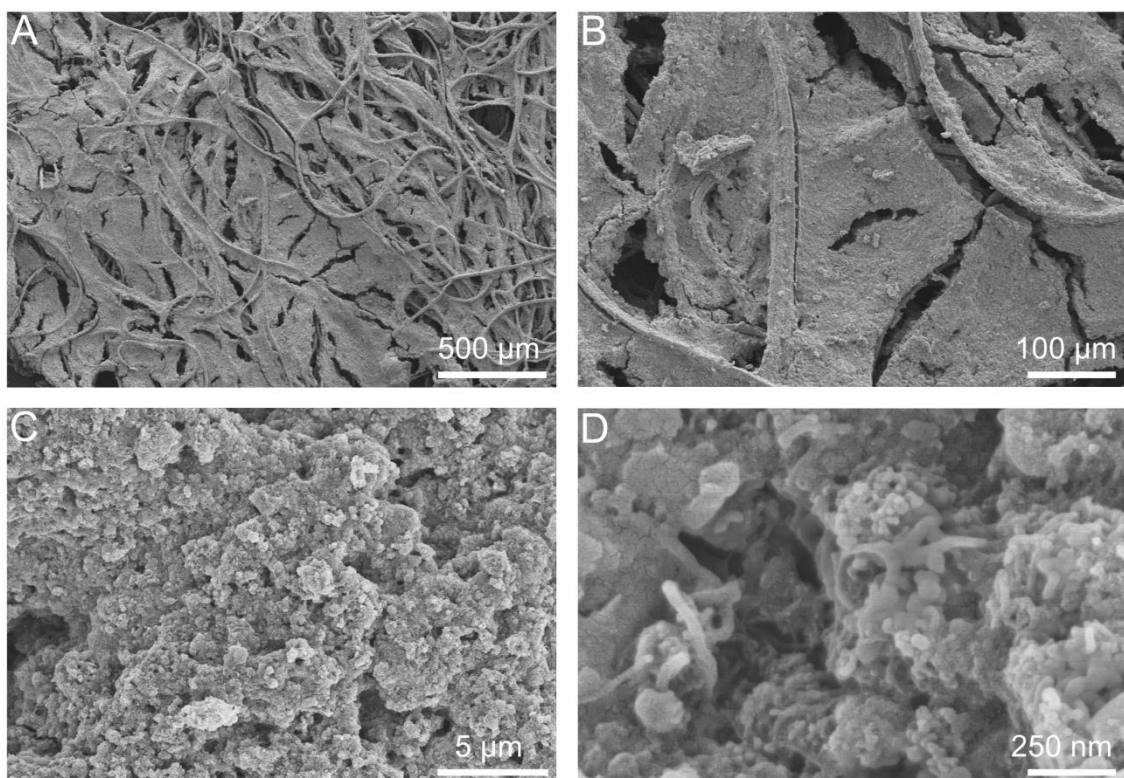
Supplementary Figure 15. (A) N₂ adsorption-desorption isotherms and pore size distribution plots using (B) DFT or (C) BJH model of OCNT_{x-y-z}.



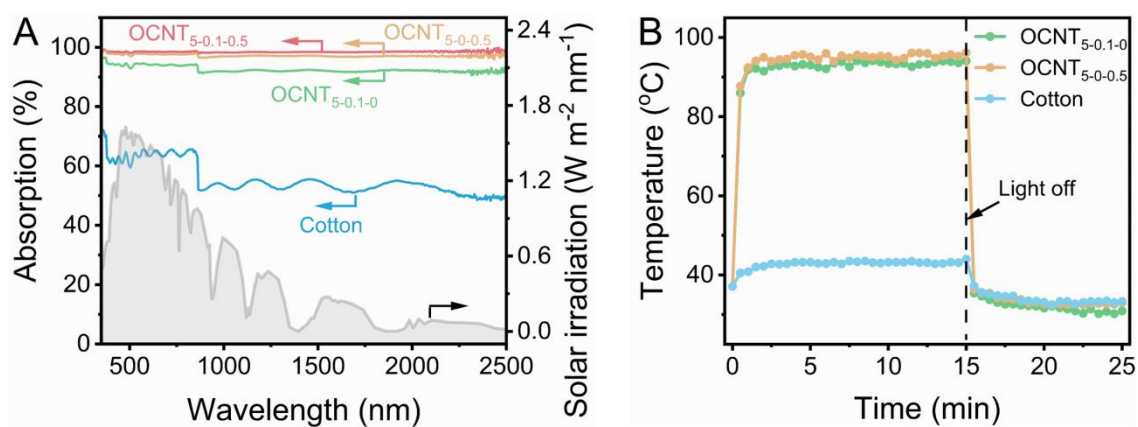
Supplementary Figure 16. (A-D) SEM images of OCNT_{5-0.1-0.5} evaporator.



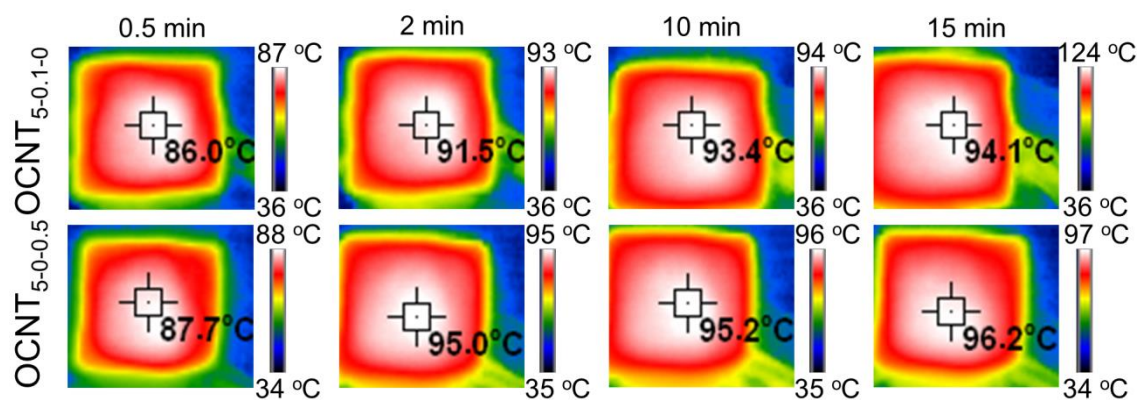
Supplementary Figure 17. (A-D) SEM images of OCNT_{5-0.1-0} evaporator.



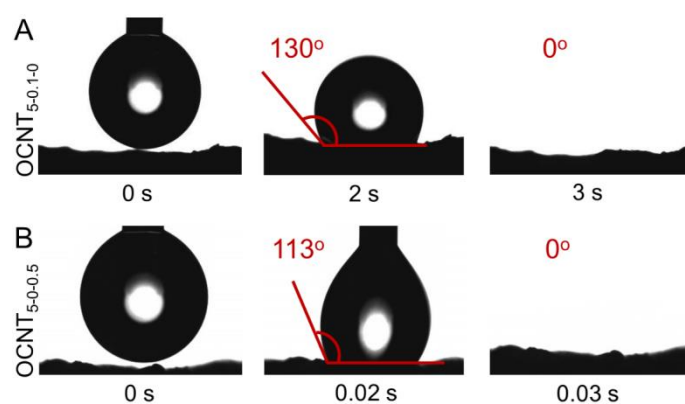
Supplementary Figure 18. (A-D) SEM images of OCNT_{5-0-0.5} evaporator.



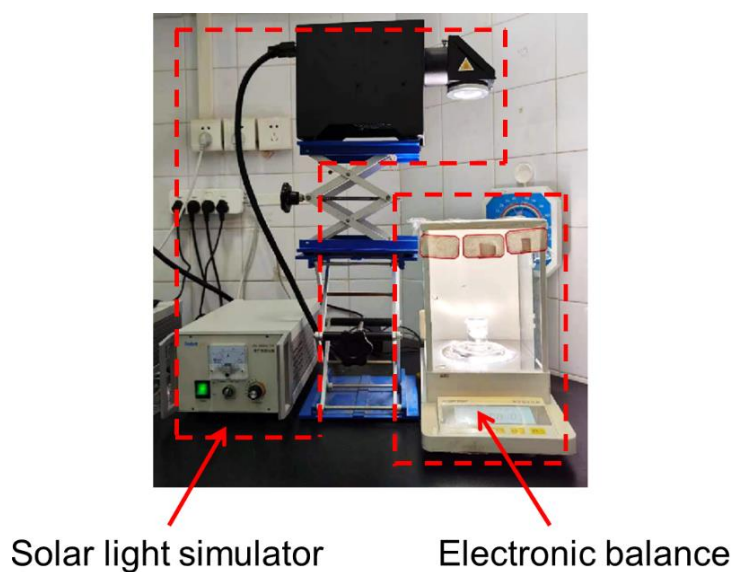
Supplementary Figure 19. (A) UV-Vis-NIR absorption spectra and (B) surface temperature curves of cotton and OCNT_{x-y-z} evaporators.



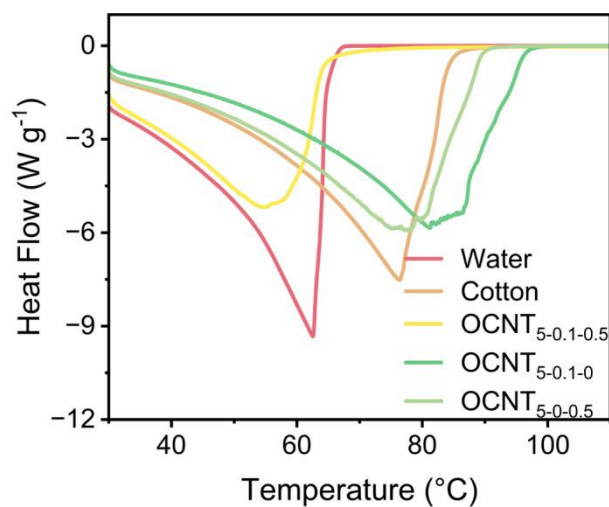
Supplementary Figure 20. Infrared images of OCNT_{5-0.1-0} and OCNT_{5-0-0.5} evaporators under 1 Sun irradiation.



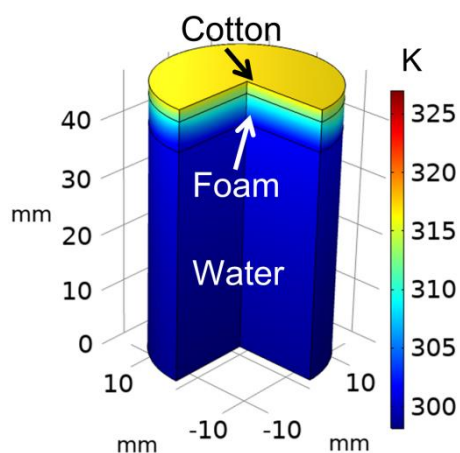
Supplementary Figure 21. Water contact angles of (A) OCNT_{5-0.1-0} and (B) OCNT_{5-0-0.5}.



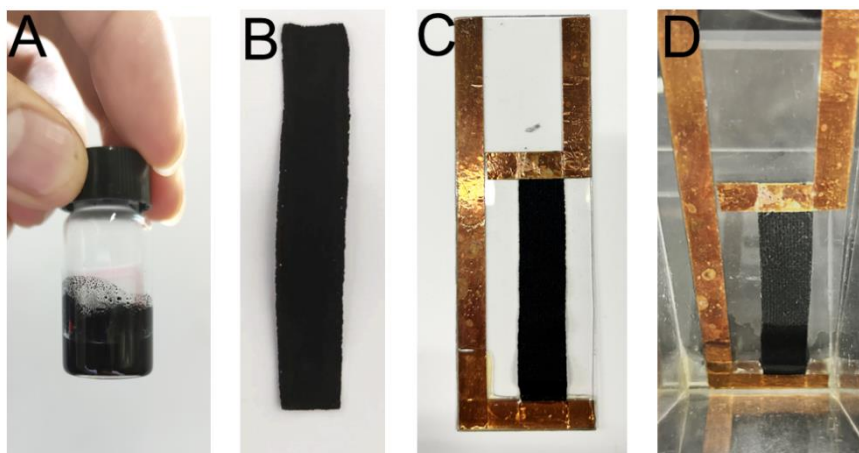
Supplementary Figure 22. Photograph of the interfacial solar evaporation system.



Supplementary Figure 23. DSC curves of water evaporation for different evaporators.



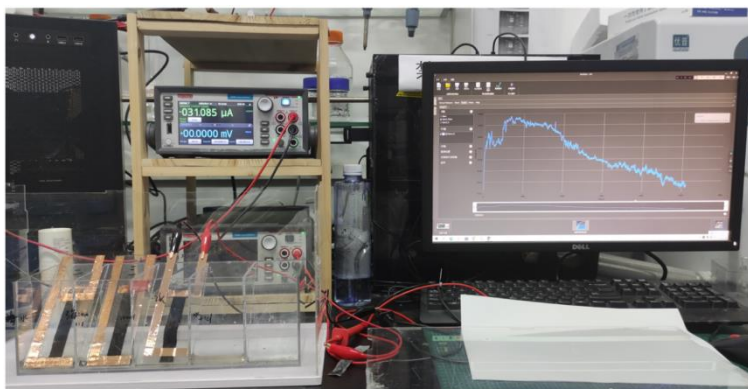
Supplementary Figure 24. COMSOL simulation of cotton evaporation system



Supplementary Figure 25. (A-D) Pictures showing the preparation process of the OCNT_{x-y-z} device.

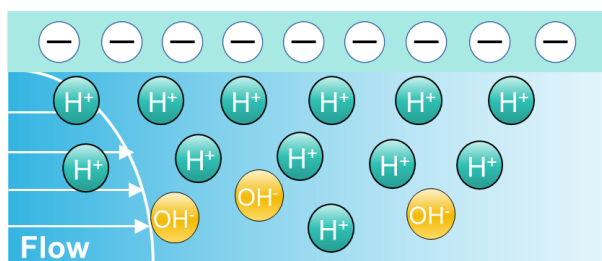
Note: Firstly, OCNT_{x-y-z} (50 mg) was added to the gelatin solution (2 wt%, 1120 μ L) and

stirred overnight at room temperature (12 h, 400 rpm, step A). Then, the mixture was spread onto cotton cloth ($1.5 \times 10 \text{ cm}^2$) and dried in the atmosphere (step B). OCNT_{x-y-z} evaporators were prepared after soaking and crosslinking with glutaraldehyde aqueous solution (5 wt%) for 5 h. Next, the OCNT_{x-y-z} evaporator was placed on the PET substrate and fixed with conductive adhesive as electrodes (step C). Finally, the connecting part of the electrode and the device was coated with epoxy resin. After drying at room temperature for 15 min, the encapsulated evaporation device was obtained.



Supplementary Figure 26. Overall diagram of water-evaporation power generation in real time.

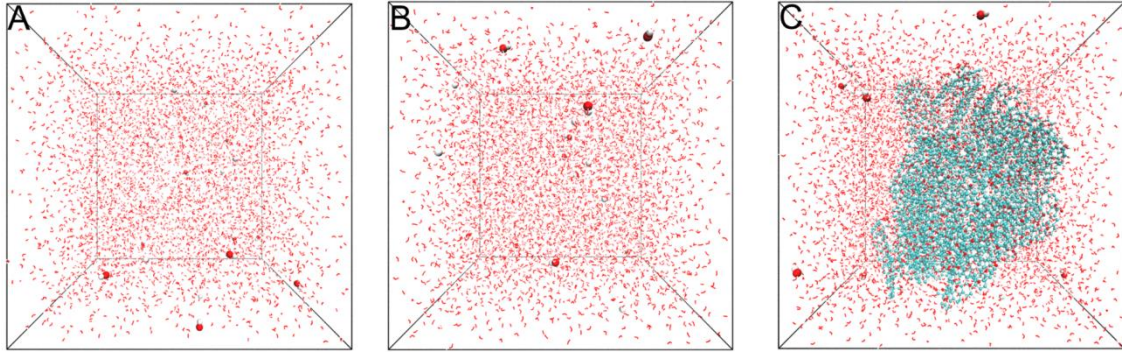
Note: The connected wire power generation device is being tested, and others are spare evaporation devices.



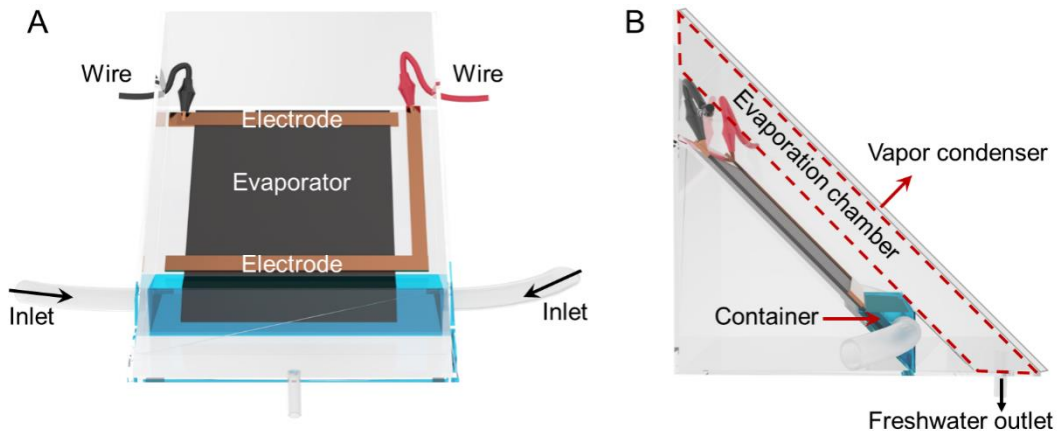
Supplementary Figure 27. Surface charge distribution model of OCNT_{5-0.1-0.5} in pure water.

Note: Oxygen-containing functional groups on OCNT_{5-0.1-0.5} surface (such as -COOH) can partially dissociate in water and generate negatively charged sites. Through electrostatic interaction, H₃O⁺ accumulates near the OCNT_{5-0.1-0.5} surface and forms an

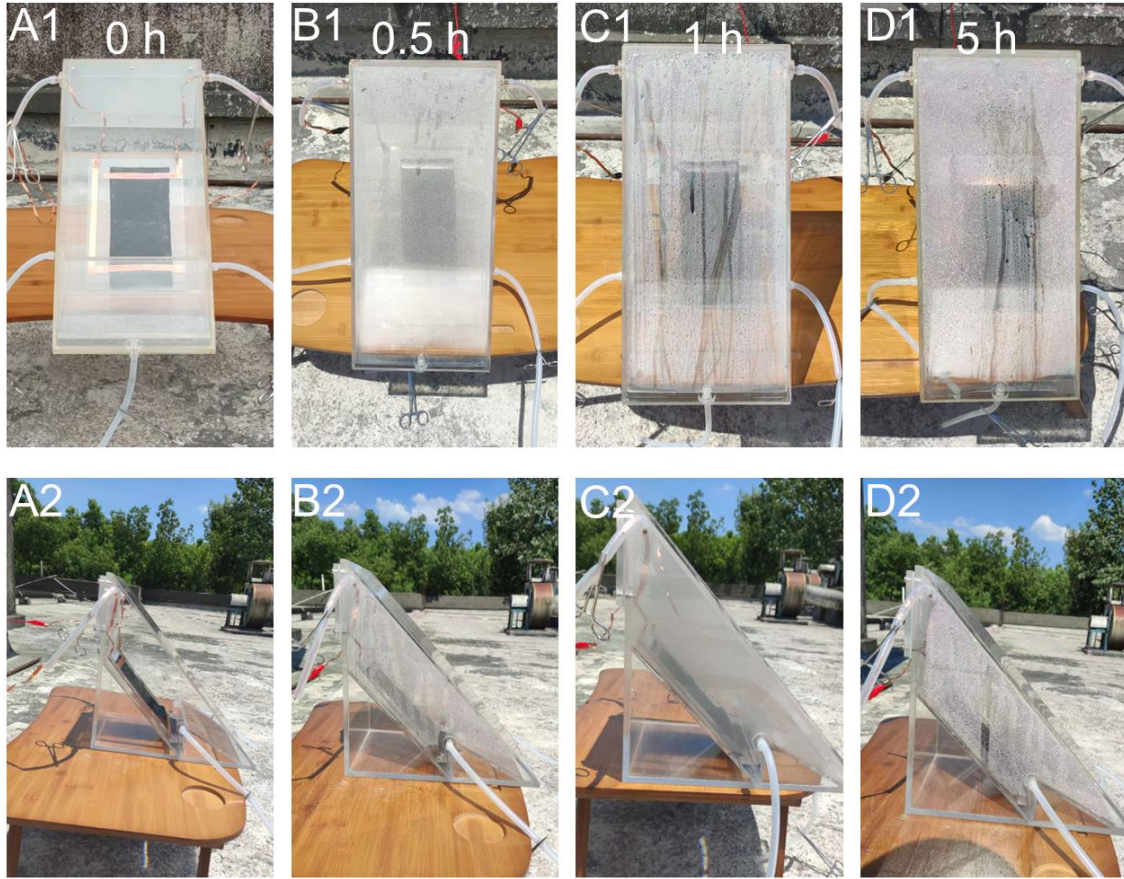
electrical double layer, whereas OH^- is repelled from the negatively charged interface. Under water evaporation-induced flow, H_3O^+ and OH^- migrate directionally at different rates, leading to the separation of ionic charge and the generation of streaming potential.



Supplementary Figure 28. Snapshot of MD simulations of (A) initial-state and (B) end-state result with pure water, and (C) end-state result with $\text{OCNT}_{5-0.1-0.5}$, H^+ , OH^- , and pure water.



Supplementary Figure 29. Scheme of the practical solar-evaporation device from (A) front view and (B) left view.



Supplementary Figure 30. Photographs of water evaporation and power generation in an outdoor experiment at different time: (A1 and A2) 0 h, (B1 and B2) 0.5 h, (C1 and C2) 1 h, and (D1 and D2) 5 h.



Supplementary Figure 31. Photograph for the series and parallel experiments of ten power generation devices to charge capacitors.

Supplementary Table 1. The material quantities added for each catalyst composition.

Catalysts	Ni(NO ₃) ₂ ·6H ₂ O (g)	(NH ₄) ₆ Mo ₇ O ₂₄ ·4H ₂ O (g)	Mg(NO ₃) ₂ ·6H ₂ O (g)	PEG-200 (g)
Ni ₅ Mo _{0.1} Mg _{0.5}	30.00	0.36	2.64	10.00
Ni ₅ Mo ₀ Mg _{0.5}	30.00	0	2.64	10.00
Ni ₅ Mo _{0.05} Mg _{0.5}	30.00	0.18	2.64	10.00
Ni ₅ Mo _{0.5} Mg _{0.5}	30.00	1.82	2.64	10.00
Ni ₅ Mo ₁ Mg _{0.5}	30.00	3.64	2.64	10.00
Ni ₅ Mo _{0.1} Mg ₀	30.00	0.36	0	10.00
Ni ₅ Mo _{0.1} Mg _{0.1}	30.00	0.36	0.53	10.00
Ni ₅ Mo _{0.1} Mg ₁	30.00	0.36	5.29	10.00
Ni ₅ Mo _{0.1} Mg ₂	30.00	0.36	10.58	10.00

Supplementary Table 2. The material quantities added in OCNT_{x-y-z} evaporators with different sizes.

Application	Area (cm ²)	OCNT _{x-y-z} (mg)	2% gelatin (μL)	Corresponding Figures
Scale-up preparation	176.62	588	13202	Figure 4A
Water evaporation indoor	6.15	20.5	460	Figure 5A, Supplementary Figure 22
Power generated indoor	15	50	1120	Figure 6A, Supplementary Figure 25
Practical experiment	200	666	14949	Figure 7A, Supplementary Figure 30

Supplementary Table 3. Comparison of the interfacial solar steam generation performance of OCNT_{5-0.1-0.5} evaporator with recently reported photothermal materials under 1 kW m⁻² irradiation.

Entry	Photothermal materials	Evaporation flux (kg m ⁻² h ⁻¹)	Efficiency (%)	Reference in Supplementary Material
1	OCNT _{5-0.1-0.5} evaporator	2.73	95.4	This work
2	CCN evaporator	2.70	98.6	[1]
3	PCC-800	2.49	90.8	[2]
4	Bi-MOF	2.16	87.5	[3]

5	CPB-PVA-5	3.50	98.5	[4]
6	ZCP-20	2.48	67.1	[5]
7	MnO/C-600 membrane	2.38	98.4	[6]
8	CSL-C@MXene-20 mg	2.35	88.2	[7]
9	CMSx aerogel	2.34	91.7	[8]
10	Plasmonic wooden flower	2.08	97	[9]
11	Sunflower stalk pith	1.9	98.8	[10]
12	Highly hydratable hydrogel network	3.18	99	[11]
13	PPy sponge	1.89	85.6	[12]
14	GCP-20	1.87	79.2	[13]
15	CDW@MOF	1.81	89	[14]
16	FR@EC/rGO	1.83	94.2	[15]
17	TPA-SBTQ	1.337	92	[16]
18	Co-MOF/CNT membrane	2.25	89.1	[17]

Supplementary Table 4. Summary of the enthalpy values measured from the dark experiment and DSC measurement.

Enthalpy (kJ g ⁻¹)	Pure water	Cotton	OCNT _{5-0.1-0.5}	OCNT _{5-0.1-0}	OCNT _{5-0-0.5}
Dark experiment	2.434	2.347	1.686	1.995	1.915
DSC measurement	2.301	2.043	1.538	1.932	1.896

Supplementary Table 5. Comparison of voltage and evaporation flux of OCNT_{5-0.1-0.5} evaporator/generator with some reported evaporators/generators.

Entry	Materials	Voltage (mV)	Evaporation flux (kg m ⁻² h ⁻¹)	Reference in SI
1	OCNT _{5-0.1-0.5}	221	2.73	This work
2	CB/PVDF	320	1.44	[18]
3	Chiber@CNT/rGO-60%	260	2.1	[19]
4	Multiwalled CNT modified wood	250	1.19	[20]
5	PCP-600 device	212	2.74	[21]
6	PCC-800	201	2.49	[2]
7	MC30	168	2.24	[22]
8	Carbon cloth	141	1.48	[23]
9	Nb ₄ N ₅ nanosheet	135	2.30	[24]
10	Carbon fiber	117	1.33	[25]
11	CNTs/carbon fiber foam	105	1.67	[26]
12	CNTP	100	1.28	[27]
13	MoS _{2-x} NSAs	98.2	1.32	[28]
14	In ₂ O ₃ /TiO ₂	80	1.51	[29]
15	MXene nanosheet	120	3.3	[30]
16	CNTs/cellulose sponge	60	1.20	[31]

Supplementary Note 1

Calculation of evaporation flux and conversion efficiency

The interfacial solar vapor generation system consisted of a solar light simulator (PLS-SXE300E), a UV reflection filter, an electronic balance (JA2003), and an infrared camera (DMI220). The surrounding temperature and relative humidity were approximately 25 °C and 33%, respectively. The infrared camera was used to collect surface temperature and thermal distribution of evaporators. Evaporation flux (m , kg m⁻² h⁻¹) and conversion efficiency (η , %) of the evaporator were calculated through Equations S1 and S2, respectively,

$$m = \Delta m / (S \times t) \quad (S1)$$

$$\eta = m' \times h_{LV} / (3600 \times P_{in}) \quad (S2)$$

where Δm stands for the water mass loss in 1 h (kg), S represents the lighting area of the evaporator (6.15×10^{-4} m²), t refers to the irradiation time (1 h), m' presents the evaporation flux that subtracts the darkroom evaporation flux, h_{LV} represents the water evaporation enthalpy (kJ kg⁻¹), and P_{in} stands for the illumination intensity (1 kW m⁻²).

Supplementary Note 2

Characterization

Scanning electron microscopy (SEM, Hitachi, SU8010, Japan) was used to investigate the morphology of OCNT_{5-0.1-0.5} and OCNT_{5-0.1-0.5} evaporator. The crystal structure was analyzed by X-ray diffraction (XRD, Rigaku, SmartLab-SE, Japan). The metallic oxide of catalysts and the crystal structure of carbon materials were analyzed by Raman spectroscopy (HORIBA Jobin Yvon, LabRAM HR800, Japan). The thermal stability of Ni₅Mo_{0.1}Mg_{0.5} and OCNT_{5-0.1-0.5} was measured by thermal gravimetric analysis (TGA, Perkin Elmer, Pyris1 TGA, China). H₂-temperature programmed reduction (H₂-TPR, JWGB, AMI-300, China) analysis was conducted with a temperature ramp of 10 °C min⁻¹ under a gas flow consisting of a mixture of hydrogen and argon (H₂:Ar = 10:90, 30 mL min⁻¹). Before the TPR evaluation, catalysts were pretreated with Ar gas at 200 °C for 1 h. During the reduction process, the amount of H₂ consumption was measured using a thermal conductivity detector (TCD). CO₂-temperature programmed desorption (CO₂-

TPD) experiments were performed on a multifunction chemisorption analyzer (JWGB, AMI-300, China). A mixture of CO₂ and He (CO₂:He = 10:90) was selected as the gas flow. The CO₂ TPD was carried out under an Ar flow of 30 mL min⁻¹ with a heating speed of 10 °C min⁻¹; the liberated CO₂ was monitored by TCD signals. The specific surface area and pore structure of OCNT_{5-0.1-0.5} were measured by the surface analyzer (Micromeritics, ASAP 2460, America). The density functional theory (DFT) model or Barret-Joyner-Halenda (BJH) model was used to determine the pore size distribution. The functional group of OCNT_{5-0.1-0.5} was analyzed by Fourier-transform infrared spectroscopy (FT-IR, BRUKER, Vertex 80, Germany) and X-ray photoelectron spectroscopy (XPS, Thermo Fisher, ESCALAB 250XI, America). Light absorption was tested via a UV-Vis-NIR spectrophotometer (Perkin Elmer, Lambda 750 S, China) within the spectral range of 300-2500 nm. The water contact angle of the OCNT evaporator was measured by micro-optical contact angle measurement instrument (Dataphysics, OCA15EC, Germany). Thermal conductivity was tested by a thermal conductivity analyzer (Hot Disk AB, TPS 2500, Sweden). The evaporation enthalpy of evaporators was analyzed by a differential scanning calorimeter (DSC, Perkin Elmer, Diamond DSC, China). The surface temperature distribution was examined using the COMSOL Multiphysics 5.6 software. Open-circuit voltage and short-circuit current were tested by a Digital SourceMeter (Beijing JKZC Technology Development Co., Ltd., Keithley 2450, China). Zeta potential was measured by using BeNano180Zeta (China).

Supplementary Note 3

Calculation of water evaporation enthalpy

The energy for water to evaporate in the dark is gained from the environment, which is therefore the same for different evaporators.

Considering theoretical evaporation enthalpy of liquid water is ca. 2.434 kJ g⁻¹. Then enthalpy values are obtained as follows,

$$U_{in}=E_{aque}m_g=E_0m_0 \quad (S3)$$

where U_{in} is the total energy absorbed from the environment per hour; E_0 and m_0

refer to the water vaporization enthalpy (2.43 kJ g^{-1}) and the water mass loss (g) of pure water without evaporators in the dark, respectively; E_{aque} is the equivalent evaporation enthalpy of the corresponding system (kJ g^{-1}), and m_g means the corresponding water mass change.

The mass loss of pure water, cotton, OCNT_{5-0.1-0.5}, OCNT_{5-0.1-0}, and OCNT_{5-0-0.5} evaporators in the dark are 295, 306, 426, 360, and 375 mg, respectively. Therefore, the water evaporation enthalpy of cotton cloth, OCNT_{5-0.1-0.5}, OCNT_{5-0.1-0}, and OCNT_{5-0-0.5} are 2.347, 1.686, 1.995 and 1.915 kJ g^{-1} , respectively, which is reduced by 3.5%, 30.7%, 18% and 21.3%, respectively, in comparison to pure water (2.434 kJ g^{-1}).

Supplementary Note 4

COMSOL simulation

The simulated 3D models were established based on the actual OCNT_{5-0.1-0.5} membrane evaporation system, which mainly consisted of OCNT_{5-0.1-0.5} membrane, PS foam, and bulk water. The upper hollow cylinder with 2 mm in height and 15 mm in radius was simulated to the membrane evaporator, the middle core cylinder with 3 mm in height and 15 mm in radius was simulated to the floating PS foam, and the remainder of a whole cylinder with 40 mm in height and 15 mm in radius was simulated to the bulk water. Subsequently, the temperature distribution was described as the following equations,

$$E_{in} = \rho C_P \frac{\partial T}{\partial t} + \rho C_P u \cdot \nabla T + \nabla q \quad (\text{S4})$$

$$q = -k \nabla T \quad (\text{S5})$$

where E_{in} is the thermal energy input from the solar irradiation; $T(x, t)$ refers to the local temperature; x and t are the space vector and time, respectively; ρ , C_P and k are the mass density, specific thermal capacity, and thermal conductivity of the evaporator, respectively; u is the fluid flow speed of the aqueous medium.

The theoretical simulation was performed by COMSOL Multiphysics 5.6 under the steady-state analysis mode. The environment temperature was set to 298.15 K, and the heat convection between the upper surface of evaporator and air was corrected by Newton's law of cooling. The thermal conductivity, density, and specific thermal

capacity of cotton cloth are $0.0674 \text{ W m}^{-1} \text{ K}^{-1}$, 67 kg m^{-3} , and $4025.43 \text{ J kg}^{-1} \text{ K}^{-1}$, respectively. The thermal conductivity, density, and specific thermal capacity of OCNT_{5-0.1-0.5} are $0.0752 \text{ W m}^{-1} \text{ K}^{-1}$, 101 kg m^{-3} , and $2658.27 \text{ J kg}^{-1} \text{ K}^{-1}$, respectively. The thermal conductivity, density, and specific thermal capacity of PS foam are $0.03 \text{ W m}^{-1} \text{ K}^{-1}$, 30 kg m^{-3} , and $1300 \text{ J kg}^{-1} \text{ K}^{-1}$, respectively.

Supplementary Note 5

Analyses of heat loss

Normally, the heat loss of water evaporation process includes radiation, convection, and conduction. The calculating details of heat loss are shown as follows,

(1) Heat radiation

The heat radiation loss was calculated by the Stefan-Boltzmann equation,

$$\Phi = \varepsilon A \sigma (T_1^4 - T_2^4) \quad (\text{S6})$$

where Φ represents the heat flux, ε is the emissivity, and the emissivity in the water evaporation processes is supposed to have a maximum emissivity of 1. A is the effective evaporation surface area ($6.16 \times 10^{-4} \text{ m}^2$). σ is the Stefan-Boltzmann constant (the value is $5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$). T_1 is the surface temperature of the materials after stable steam generation under one-sun illumination (ca. 55.6°C , 328.75 K), and T_2 is the ambient temperature upward of the absorber (ca. 39.4°C , 312.55 K). Then using the following equation to calculate the radiation loss,

$$\eta_{rad} = \Phi / P_{in} \quad (\text{S7})$$

Therefore, the calculated heat radiation loss of the OCNT_{5-0.1-0.5} evaporator is 7.5%.

(2) Heat convection

The convective heat loss is defined by Newton's law of cooling as shown below,

$$Q = h A \Delta T \quad (\text{S8})$$

where Q is the convection heat flux, h represents the convection heat transfer coefficient, which is approximately $5 \text{ W m}^{-2} \text{ K}^{-1}$. ΔT is the difference between the surface temperature of OCNT_{5-0.1-0.5} evaporator and the ambient temperature upward the absorber. Consequently, the connection heat loss of the OCNT_{5-0.1-0.5} evaporator was calculated

through Equation S8, and the value is 4.9%.

(3) Heat conduction

$$Q=Cm\Delta T \quad (S9)$$

where Q is the heat energy, C presents the specific heat capacity of water ($4.2 \text{ kJ K}^{-1} \text{ kg}^{-1}$), and m denotes the weight of water (g). ΔT is the increased temperature of water. In this work, $m = 35 \text{ g}$, $\Delta T = 0.5 \text{ K}$, Consequently, according to Equation S9, the calculated conduction heat loss of the OCNT_{5-0.1-0.5} evaporator is ca. 3.3%.

Therefore, the heat loss of the OCNT_{5-0.1-0.5} evaporator in the water evaporation is ca. 15.7%.

Supplementary Note 6

Theoretical calculation

The size of OCNT_{5-0.1-0.5} synthesized in the experiment is too large, and single-side graphene oxide (GO) fragments are used to simulate OCNT_{5-0.1-0.5} in the simulation calculation. The partial charge of GO with different oxygen content was calculated using Gaussian 16 code^[32] and the 6-311g (d,p) basis functions were applied^[33]. The OPLSS-AA force field^[34] and Auxiliary Tools of Force Field (AuToFF) were used to parametrize all atoms, such as bond parameters, angle parameters, and dihedral angles. The interactions of different graphene oxide with H^+ and OH^- were studied by molecular dynamics (MD) simulation. In system 1, 30 GO molecules, 10 H^+ , 10 OH^- and 5560 water molecules were randomly inserted into a cube box with a side length of 7.0 nm. The model of water molecule is TIP3P^[35]. The MD simulations were performed in the GROMACS 2021 software package^[36-38]. The steepest descent method was applied to minimize the initial energy for each system with a force tolerance of $1 \text{ kJ mol}^{-1} \text{ nm}^{-1}$ and a maximum step size of 0.002 ps before MD calculations^[39]. In all the three directions, periodic boundary conditions were imposed. Leapfrog algorithm was used to integrate the Newtonian equation of motion^[39]. The MD simulation was processed in an NPT ensemble and the simulation time is 20 ns. In system 2, 10 H^+ , 10 OH^- and 5560 water molecules were added into the simulated system. Other operation steps are the same as

the system 1.

In NPT simulations, the pressure was maintained at 1 bar by the Berendsen barostat in an isotropic manner^[40]. The temperature was maintained by the V-rescale thermostat at 298.15 K. The LINCS algorithm^[41] was performed for constrain bond lengths of hydrogen atoms. A cutoff of 1.0 nm was employed to calculate the short-range van der Waals interactions and the electrostatic interactions^[42].

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