

Supplementary Information

Wood-inspired Polypyrrole/Cellulose Aerogel with Vertically Aligned Channels Prepared by Facile Freeze-casting for Efficient Interfacial Solar Evaporation

Yuxuan Ren^a, Rufan Zhou^a, Tao G. Dong^b, Qingye Lu^{a,}*

^a Department of Chemical and Petroleum Engineering, University of Calgary, 2500 University Drive, NW, Calgary, Alberta, T2N 1N4, Canada

^b Department of Immunology and Microbiology, School of Life Sciences, Southern University of Science and Technology, Shenzhen, 518055, China

* **Corresponding author:** Qingye Lu (qingye.lu@ucalgary.ca)

Note 1: Dark Experiment for Estimation of Evaporation Enthalpy.¹⁻³

The dark experiment was carried out under room condition (temperature: around 22 °C; humidity: around 15%). Pure water was used as the reference and samples with the same evaporation area were put in a closed container and left for 24 h under dark condition. And the mass difference before and after was obtained by a balance (Mettler Toledo, ME 204). The energy input for the whole system was assumed as identical. Thus, the following equation (S1) could be used to calculate the evaporation enthalpy with materials.

$$H_w \Delta m_{w,RT} = H_s \Delta m_{s,RT} \quad \text{Equation (S1)}$$

where H_w and H_s are evaporation enthalpy for bulk water and water with samples, respectively; $\Delta m_{w,RT}$ and $\Delta m_{s,RT}$ are mass change of bulk water and water with samples at room temperature, respectively.

The evaporation enthalpy for bulk water under different temperature was calculate by following equation (S2):⁴

$$H_w = 1.91846 \times 10^{-6} \times \left(\frac{T}{T-33.91}\right)^2 \quad \text{J/kg} \quad \text{Equation (S2)}$$

where T is the temperature when evaporation happens (K). Based on Equation S1 and S2, the water evaporation enthalpy with samples under different temperatures could be estimated by following equation (S3):

$$H_s = \frac{\Delta m_{w,RT}}{\Delta m_{s,RT}} H_w = \frac{\Delta m_{w,RT}}{\Delta m_{s,RT}} \times 1.91846 \times 10^{-6} \times \left(\frac{T}{T-33.91}\right)^2 \quad \text{Equation (S3)}$$

The corresponded results of estimated evaporation enthalpy were shown in Figure 5(a).

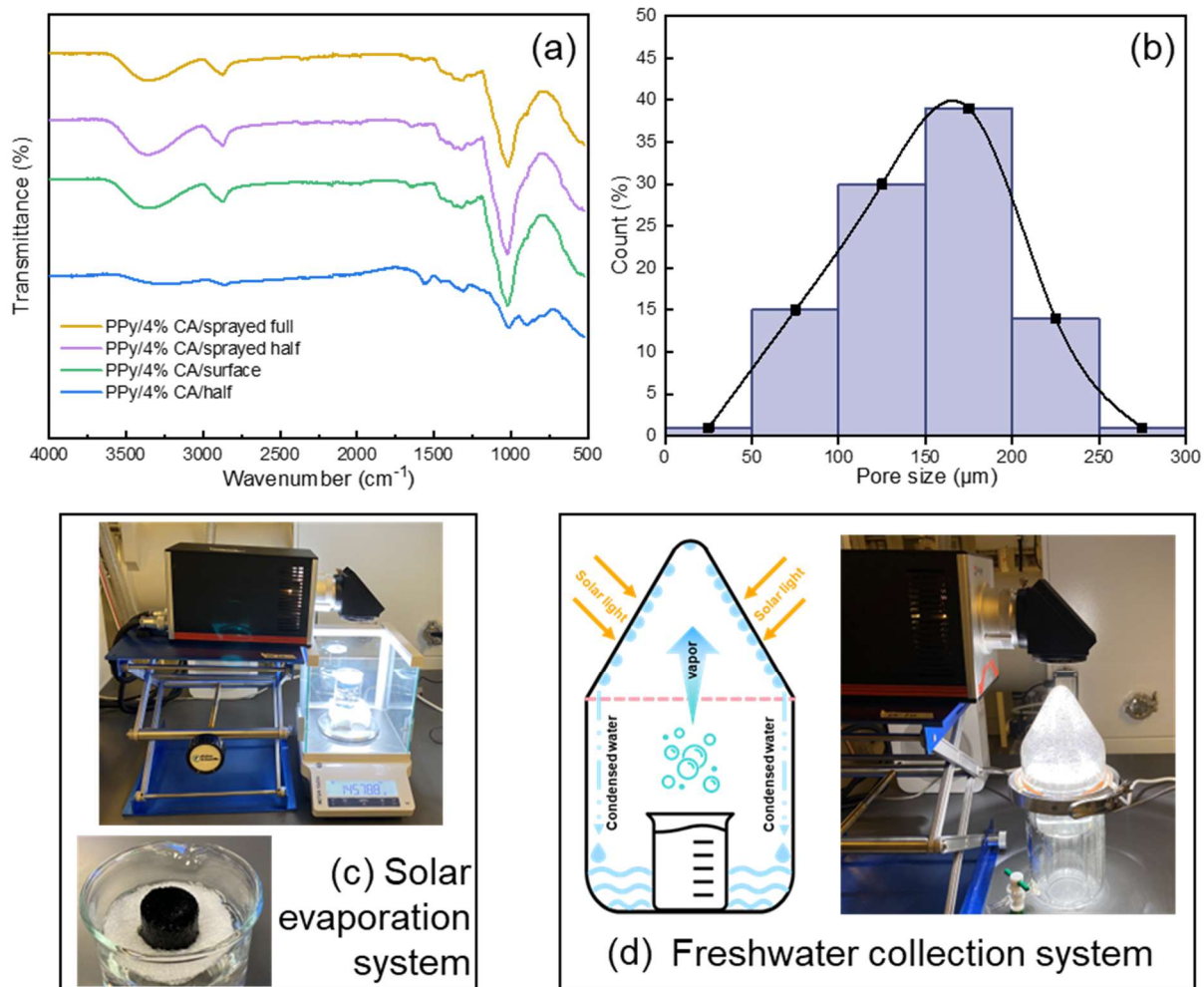


Figure S1. (a) FTIR spectrum of PPy/4% CA samples. (b) Size distribution of pores of 4% CA. (c) Photograph of solar evaporation system. (d) Schematic and photograph of freshwater collection system.

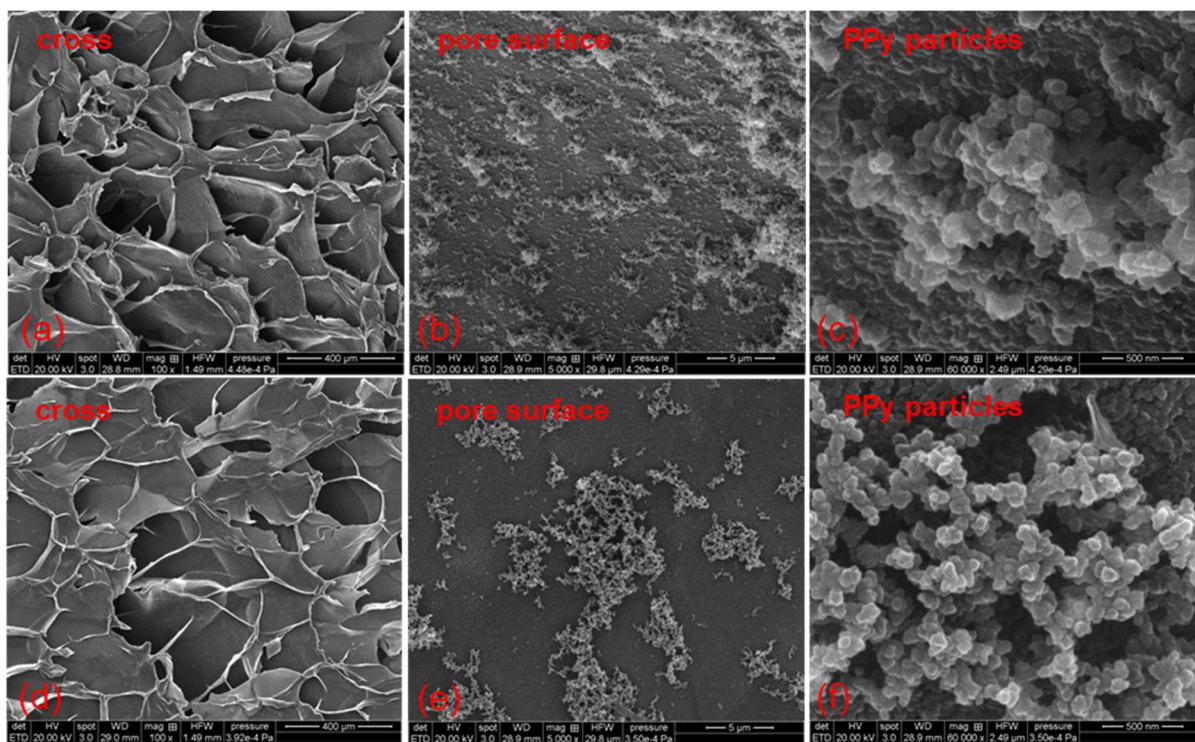


Figure S2. SEM images of PPy/4% CA/half (a, b, c) and PPy/4% CA/surface (d, e, f).

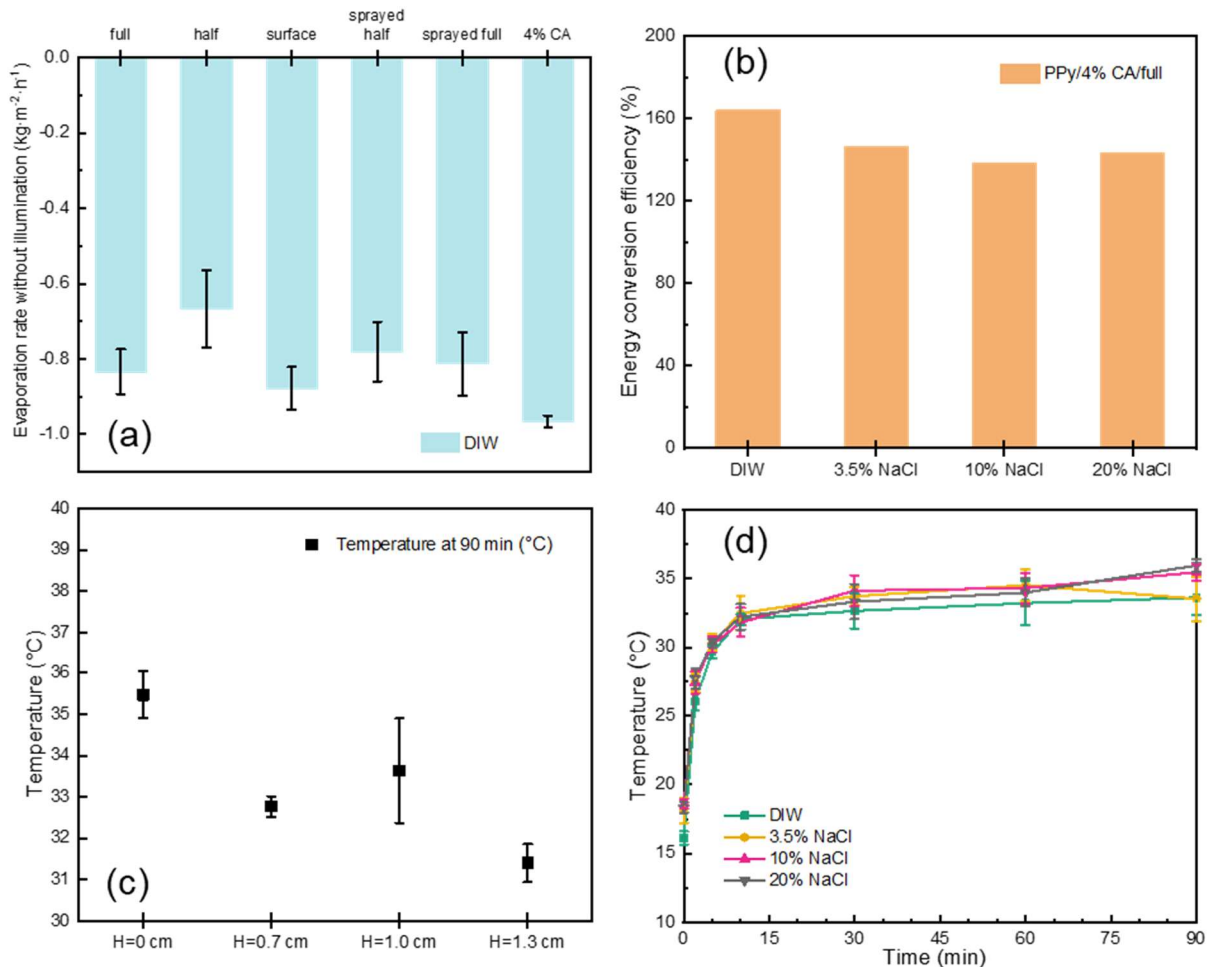


Figure S3. (a) Evaporation rate of different samples without illumination ($H=1$ cm). (b) Energy conversion efficiency under one sun illumination in different saline concentrations calculated by using enthalpy of bulk water (sample: PPy/4% CA/full; $H=1$ cm). (c) Stabilized surface temperature of PPy/4% CA/full of different exposure heights. (d) Temperature change of PPy/4% CA/full in NaCl solution with different concentrations ($H=1$ cm).

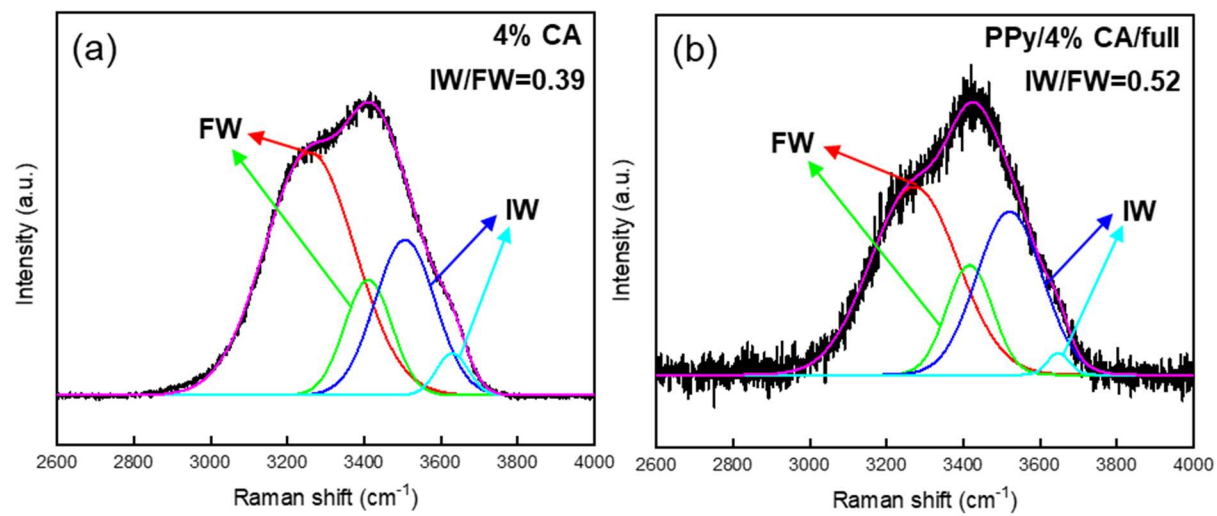


Figure S4. Raman spectrum with fitted peaks of (a) 4% CA and (b) PPy/4% CA/full at fully swollen state.

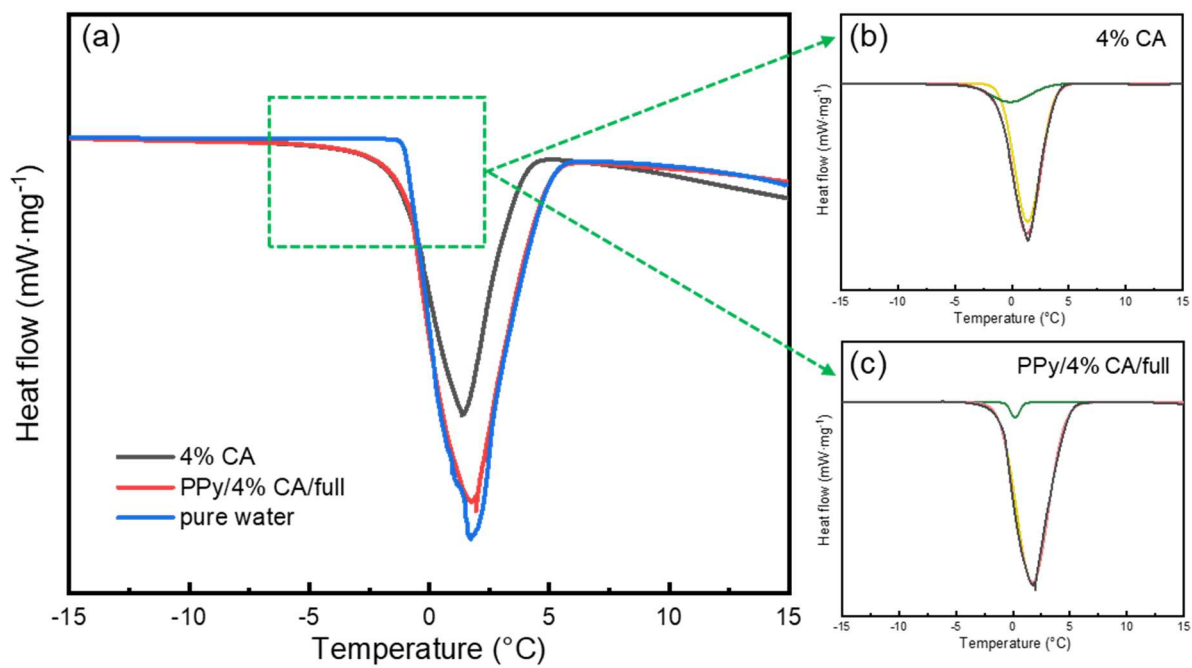


Figure S5. (a) DSC curves of different samples at fully swollen state. Fitted DSC curve of (b) 4% CA and (c) PPy/4% CA/full at fully swollen state.

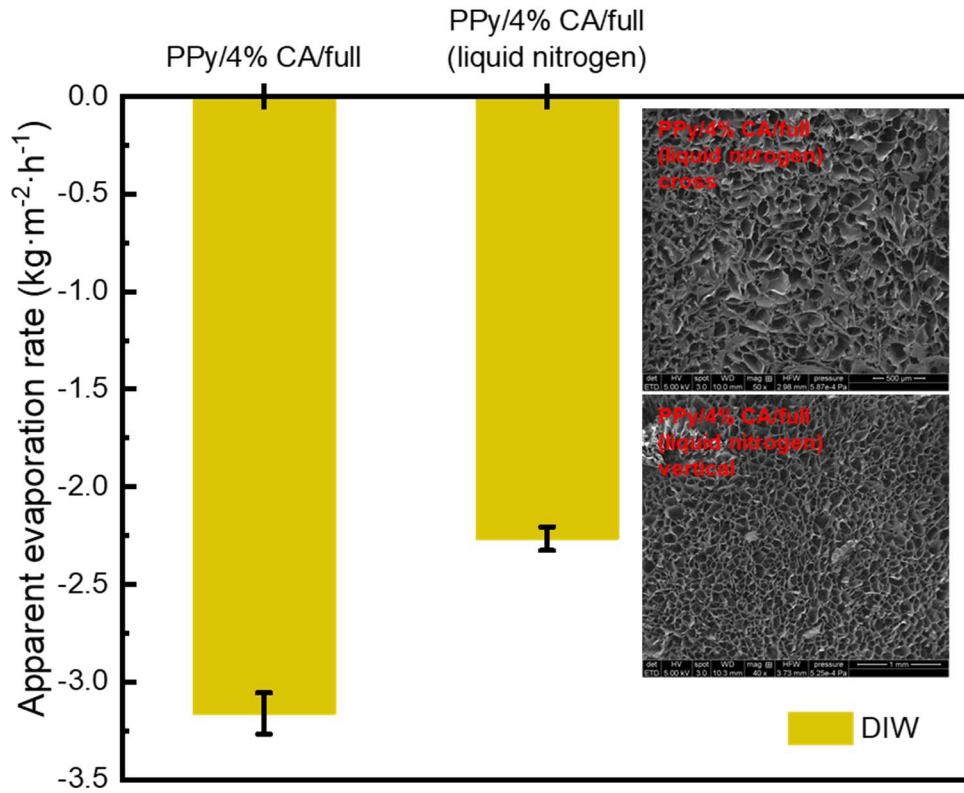


Figure S6. Evaporation performance comparison between PPy/4 %CA/full prepared by freeze-casting (with vertical structure) and liquid nitrogen frozen (without vertical structure) with inserted SEM images of PPy/4 %CA/full prepared by liquid nitrogen frozen from cross and vertical directions.

Note 2: An outdoor one-month stability test in 3.5% NaCl solution of PPy/4% CA/full.⁵

PPy/4% CA/full was put in the 3.5% NaCl solution outdoor for 30 days and the evaporation performance was tested under one sun illumination using AULIGHT xenon lamp system (PE300L-3A, equipped with an AM 1.5G optical filter) for 1 h everyday. After testing, the aerogel was put back to 3.5% NaCl solution outdoor again. During the 1-h testing, the humidity was recorded as well.

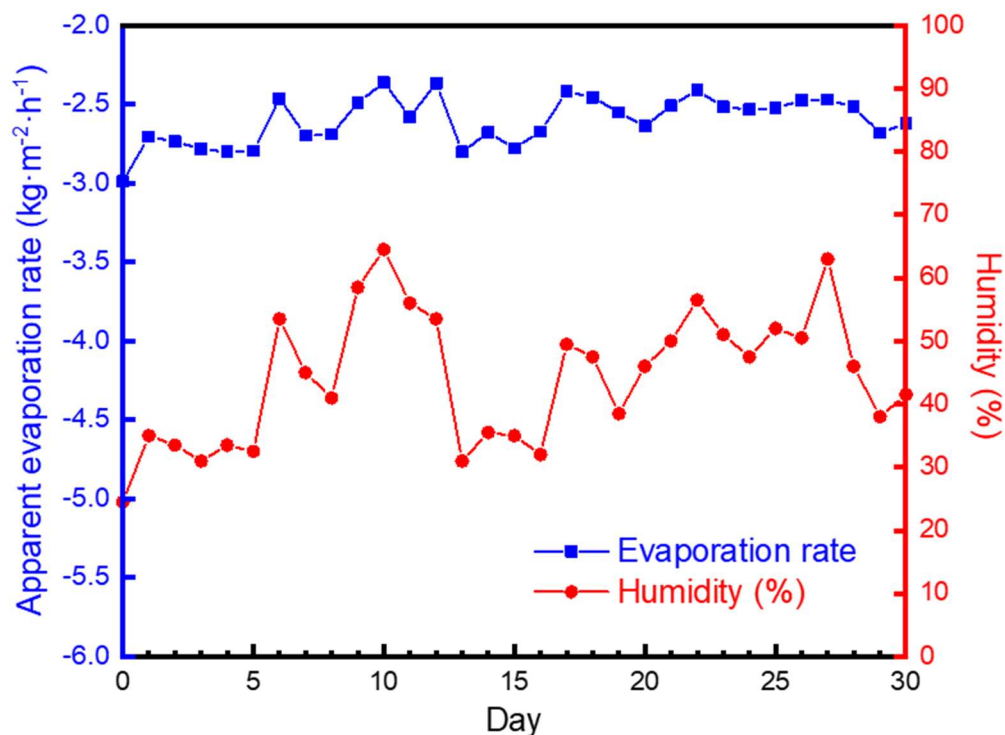


Figure S7. One-month stability test of PPy/4% CA/full in 3.5% NaCl solution (outdoor) with humidity (at testing time) included.

Table S1. Summary of aerogel solar evaporators.

Material	Cellulose source	Preparation method	Evaporation rate (kg·m ⁻² ·h ⁻¹) (1 sun)	Saline/wastewater treatment
PPy/CA (This work)	Cellulose microcrystalline powder	<i>In-situ</i> synthesis of PPy on CA	3.16 (H=1 cm)	High purity of condensed water from seawater and wastewater containing dyes and heavy metals.
CuS/BC bi-layered foam ⁶	Bacterial cellulose	<i>In-situ</i> synthesis of CuS/BC photothermal layer, followed by crosslinking fresh BC precursor	1.44 (3.5% NaCl)	Self-floating, self-cleaning, simultaneously photocatalytic degradation of MB
PPy/TOCNFA ⁷	TEMPO-oxidized cellulose nanofibrils	Directional stabilization by electrostatic interaction and drying at ambient condition, followed by <i>in-situ</i> growth of PPy	1.32	High purity of condensed water from seawater.
PPy/CA ⁸	cotton linter pulp	Bi-layered structure with PPy synthesized on cellulose hydrogel, then freeze-dried	1.42 (seawater)	High purity of condensed water from wastewater containing dyes and simulated seawater.
PDA/CA ⁹	cotton	Alkaline dissolving and ECH crosslinking, followed by <i>in-situ</i> growth of PDA	1.36 (seawater)	High purity of condensed water from seawater. Good adsorption of MB and RhB.
PDA/CA ¹⁰	waste cotton	One-pot synthesis in alkaline solution	2.74 (H=3 cm)	High purity of condensed water from wastewater containing dyes and simulated seawater.
CB/CNFA ¹¹	Bacterial cellulose nanofibrils	One-pot synthesis of CB/CNFA photothermal layer, followed by template-assisted core (hydrophilic)-shell (hydrophobic) CNFA	1.82	Good resistance towards different pH. High purity of condensed water from seawater. The evaporator could be used to detect water wave.
PEI@CNTs/CNFA ¹²	Textile waste cotton	One-pot synthesis in alkaline solution	1.9	High purity of condensed water from wastewater containing dyes, metal ions and simulated seawater.

CNT/CA ¹³	waste cotton fabric	Fresh cellulose suspension followed by put MTMS-treated CNT/CA as photothermal layer	1.81	High purity of condensed water from wastewater containing dyes and simulated seawater.
POTS treated CS cloth/PE/CA ¹⁴	Wood cellulose nanofibers	Flame-burned cotton cloth followed by POTS treatment, wrapping it on cotton cloth covered PE/CA prepared by Pickering emulsion freeze-drying	1.282 (3.5 wt% NaCl)	Stable performance in various water sources. High purity of condensed water from wastewater containing dyes, metal ions and NaCl solution.
RGO/SA/CA ¹⁵	Cellulose fibers from rice straw biomass	One pot synthesis crosslinked by Ca ²⁺	2.25 (H=3 cm)	High purity of condensed water from seawater.
PPy/PEI/A-CNFA ¹⁶	Aldehyde-based cellulose nanofibers	Schiff base reaction followed by In-situ synthesis of PPy	1.66	Superelastic, low thermal conductivity, high purity of condensed water from seawater and wastewater containing dyes and heavy metals.
MXene/ZIF-67/CA ¹⁷	2,2,6,6-tetramethylpiperidine-1-oxyl oxidized cellulose nanofibers	One pot synthesis of Co ²⁺ /MXene/TOCNF hydrogel followed by in-situ growth of ZIF-67	2.034	High purity of condensed water from seawater and wastewater containing heavy metals. Good flame retardant.
Ti ₃ C ₂ T _x MXene/CNFA ¹⁸	Cellulose nanofibrils	Frozen CNF-ECH, followed by one-pot precursor of MXene/CNF/ECH/M TMS, freeze-casting/drying	2.287	High purity of condensed water from saline water.
graphene aerogel ¹⁹			2.17	High purity of condensed water from saline water. It could generate electricity as well.
carbonized carbon dot/starch aerogel ²⁰			2.29	Stable performance in saline water, water with different pH values and wastewater containing MB.

rGO/PPy aerogel ²¹			2.08	High purity of condensed water from simulated seawater, wastewater containing organic contaminants. The aerogel could photodegrade organic contaminants in the wastewater.
PDA/PVA aerogel ²²			2.94 (25 wt% NaCl)	The salt could be precipitated on the tip of the evaporator.
MOF-derived MoC/C/CMC/CMC-Na aerogel ²³			2.41	Stable performance in saline water, high purity of condensed water from seawater.

References:

- 1 Z. Yu, R. Gu, Y. Zhang, S. Guo, S. Cheng and S. C. Tan, *Nano Energy*, 2022, **98**, 107287.
- 2 Q. Lu, W. Shi, H. Yang and X. Wang, *Advanced Materials*, 2020, **32**, 2001544.
- 3 X. Zhou, F. Zhao, Y. Guo, B. Rosenberger and G. Yu, *Sci Adv*, , DOI:10.1126/sciadv.aaw5484.
- 4 T. Hu, L. Li, Y. Yang and J. Zhang, *J Mater Chem A Mater*, 2020, **8**, 14736–14745.
- 5 Q. Zhao, Z. Wu, X. Xu, R. Yang, H. Ma, Q. Xu, K. Zhang, M. Zhang, J. Xu and B. Lu, *Sep Purif Technol*, 2022, **300**, 121889.
- 6 D. Zhang, M. Zhang, S. Chen, Q. Liang, N. Sheng, Z. Han, Y. Cai and H. Wang, *Desalination*, 2021, **500**, 114899.
- 7 J. Li, S. Chen, X. Li, J. Zhang, H. Nawaz, Y. Xu, F. Kong and F. Xu, *Chemical Engineering Journal*, 2023, **453**, 139844.
- 8 M. Wang, G. Xu, Z. An, K. Xu, C. Qi, R. Das and H. Zhao, *Sep Purif Technol*, 2022, **287**, 120534.
- 9 Y. Zou, J. Zhao, J. Zhu, X. Guo, P. Chen, G. Duan, X. Liu and Y. Li, *ACS Appl Mater Interfaces*, 2021, **13**, 7617–7624.
- 10 H. Liu, M. K. Alam, M. He, Y. Liu, L. Wang, X. Qin and J. Yu, *ACS Appl Mater Interfaces*, 2021, **13**, 49860–49867.
- 11 N. Li, L. Qiao, J. He, S. Wang, L. Yu, P. Murto, X. Li and X. Xu, *Adv Funct Mater*, 2021, **31**, 2008681.
- 12 M. He, Md. K. Alam, H. Liu, M. Zheng, J. Zhao, L. Wang, L. Liu, X. Qin and J. Yu, *Composites Communications*, 2021, **28**, 100936.

- 13 M. K. Alam, M. He, W. Chen, L. Wang, X. Li and X. Qin, *ACS Appl Mater Interfaces*, 2022, **14**, 41114–41121.
- 14 F. Peng, J. Xu, X. Bai, G. Feng, X. Zeng, M. R. Ibn Raihan and H. Bao, *Solar Energy Materials and Solar Cells*, 2021, **221**, 110910.
- 15 D. P. Storer, J. L. Phelps, X. Wu, G. Owens, N. I. Khan and H. Xu, *ACS Appl Mater Interfaces*, 2020, **12**, 15279–15287.
- 16 R. Zhu, D. Wang, J. Xie, Y. Liu, M. Liu and S. Fu, *Chemical Engineering Journal*, 2022, **427**, 131618.
- 17 K. Zhou, L. Yin, K. Gong and Q. Wu, *Chemical Engineering Journal*, 2023, **464**, 142616.
- 18 X. Han, S. Ding, L. Fan, Y. Zhou and S. Wang, *J Mater Chem A Mater*, 2021, **9**, 18614–18622.
- 19 Y. Xu, S. Dong, Y. Sheng, C. Liu, F. Xing, Y. Di and Z. Gan, *J Mater Chem A Mater*, 2023, **11**, 1866–1876.
- 20 X. Xu, Q. Chang, C. Xue, N. Li, H. Wang, J. Yang and S. Hu, *J Mater Chem A Mater*, 2022, **10**, 11712–11720.
- 21 S. Yan, H. Song, Y. Li, J. Yang, X. Jia, S. Wang and X. Yang, *Appl Catal B*, 2022, **301**, 120820.
- 22 Z. Huang, J. Wei, Y. Wan, P. Li, J. Yu, J. Dong, S. Wang, S. Li and C. Lee, *Small*, 2021, **17**, 2101487.
- 23 F. Yu, J. Wang, L. Yan, Z. Guo, Z. Chen, M. S. Irshad, J. Qian, T. Mei and X. Wang, *Solar Energy Materials and Solar Cells*, 2022, **243**, 111738.