

ANISOTROPIC COMPOSITE AEROGELS FOR SOLAR VAPOR GENERATION

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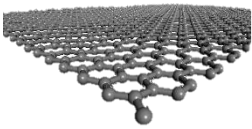
Outline

- Background and motivation
- Concept of **rational design** for anisotropic nanocomposites
- Design of anisotropic **MXene aerogels** for solar vapor generation
- Conclusions

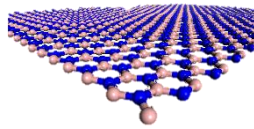
Nanocomposites: emerging materials for thermal energy regulation

Two-dimensional (2D) nanofillers

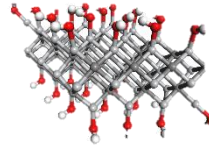
Graphene



Boron nitride

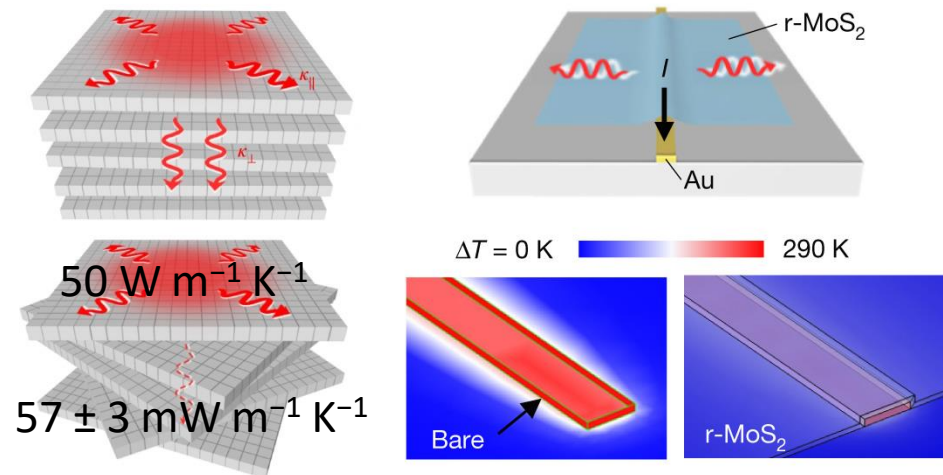


MXene



- One/few atomic layer
- High **aspect ratio**
- Large lateral size
- Large **surface area**

Anisotropic thermal conduction



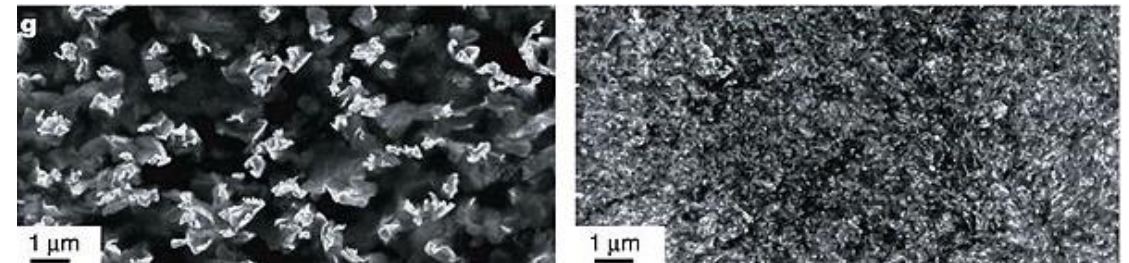
Kim et al. *Nature* **597**, 660–665 (2021)

Conventional processing technique

Dispersion → Mixing → Forming



Randomly dispersed nanofillers in matrix

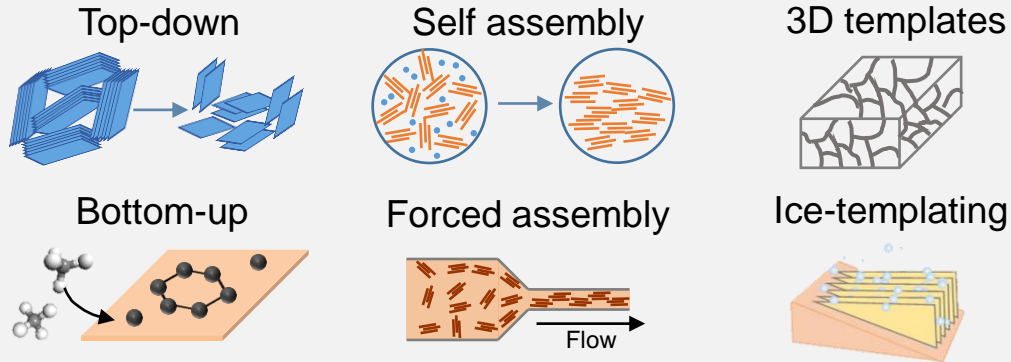


Stankovich et al. *Nature* **442**, 282–286 (2006)

How to rationally translate the anisotropic properties to bulk composites?

Rational design through multiscale modeling and controlled assembly

Controlled assembly



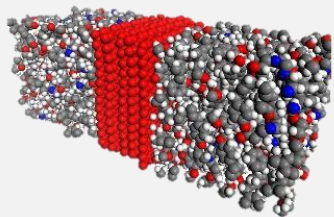
Nanoscale:
1 to 100 nm

Microscale:
0.1 to 100 μm

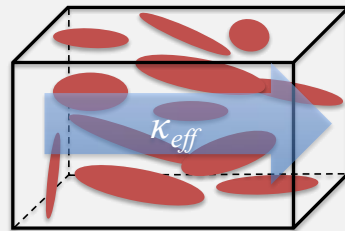
Macroscale:
>100 μm

Multiscale modeling

Molecular dynamics (MD)

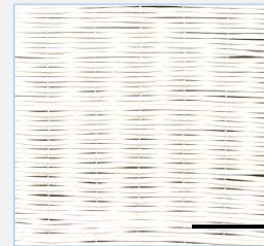


Analytical models

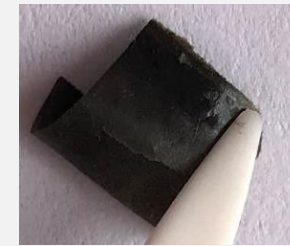


Bulk composites
with controlled multiscale structures

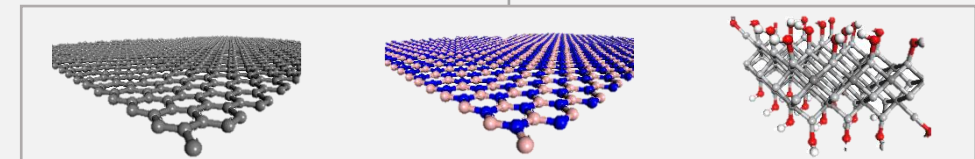
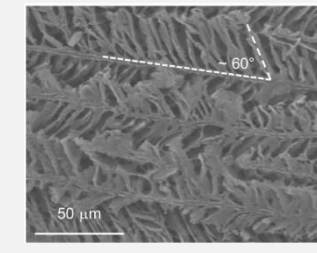
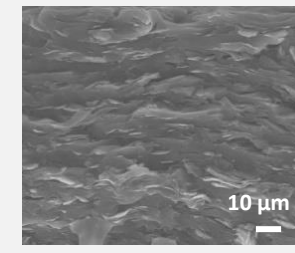
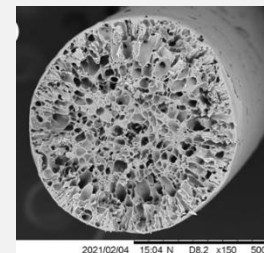
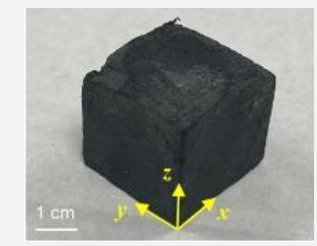
1D fiber



2D film



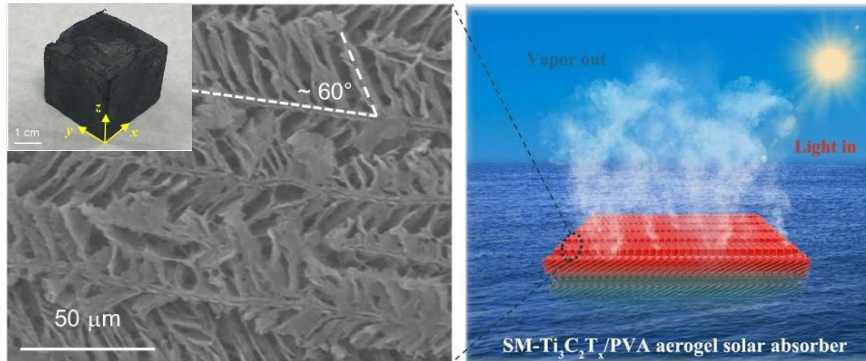
3D architecture



Shen, Zheng, Kim. *Progress in Materials Science*, 2021, 115, 100708.

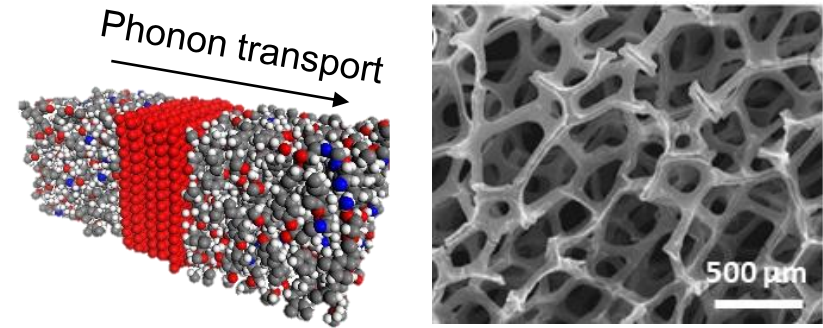
Tailored multifunctionalities for thermal management

MXene aerogels for solar-thermal heating



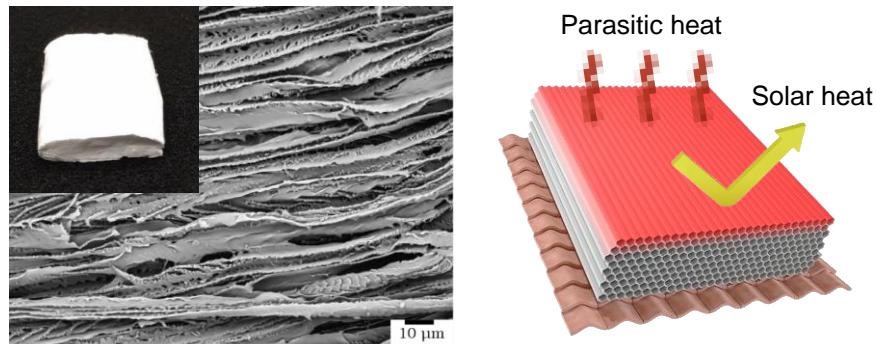
Advanced Functional Materials, 2022

Graphene/polymer composites for Thermal interfaces



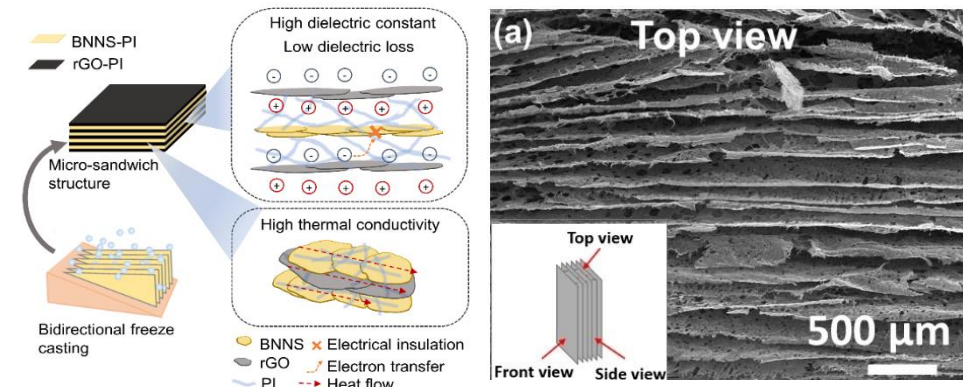
Nano lett 2016; *Mater. Horizons* 2018

BNNS aerogels for energy-efficient cooling



Nature communications 2022; *Nano-micro letters* 2022

Boron nitride/graphene films for dielectrics



Adv. Funct. Mater. 2020

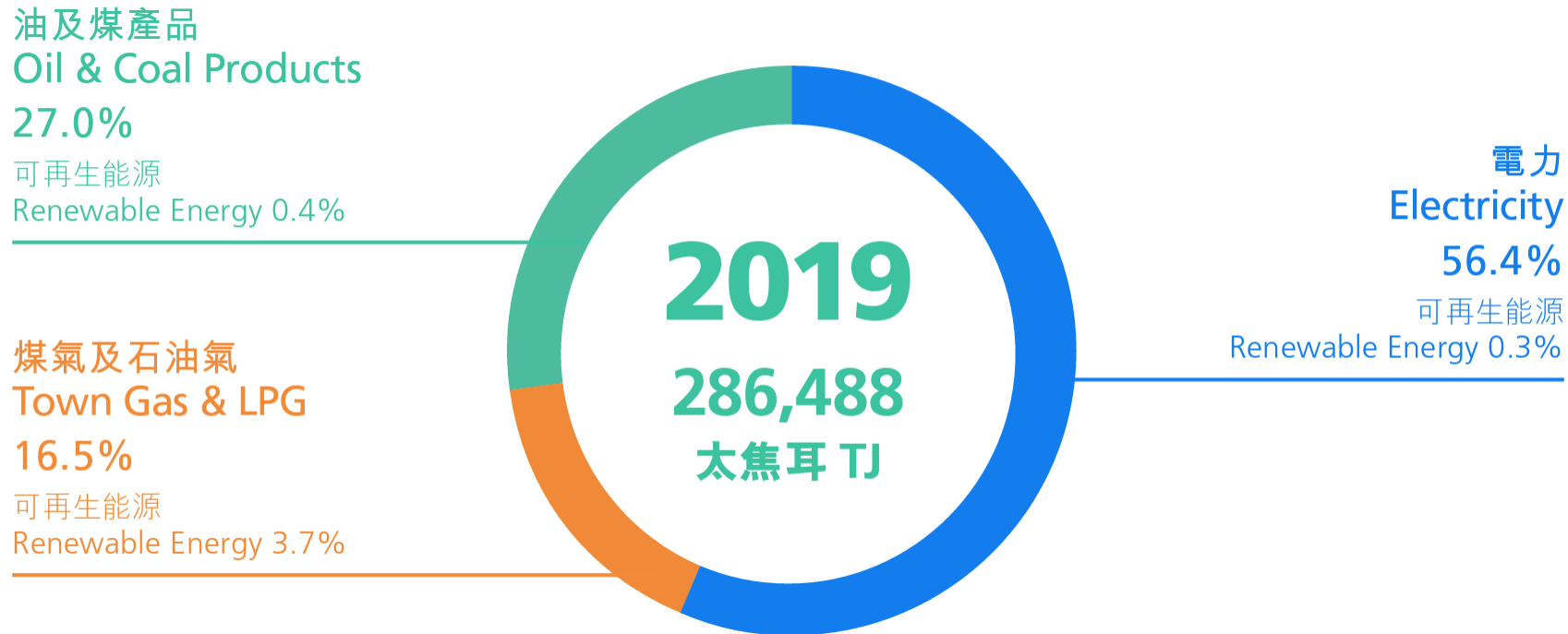
Solar absorption

Electrical conductivity

Thermal conductivity

MXene aerogels for solar vapor generation

- Renewable electricity accounts for **only 0.3%** of the "Electricity" generation
- Includes **solar energy** used to generate **electricity** by PV panels
- **Solar energy** is abundant but has **not been fully utilized**

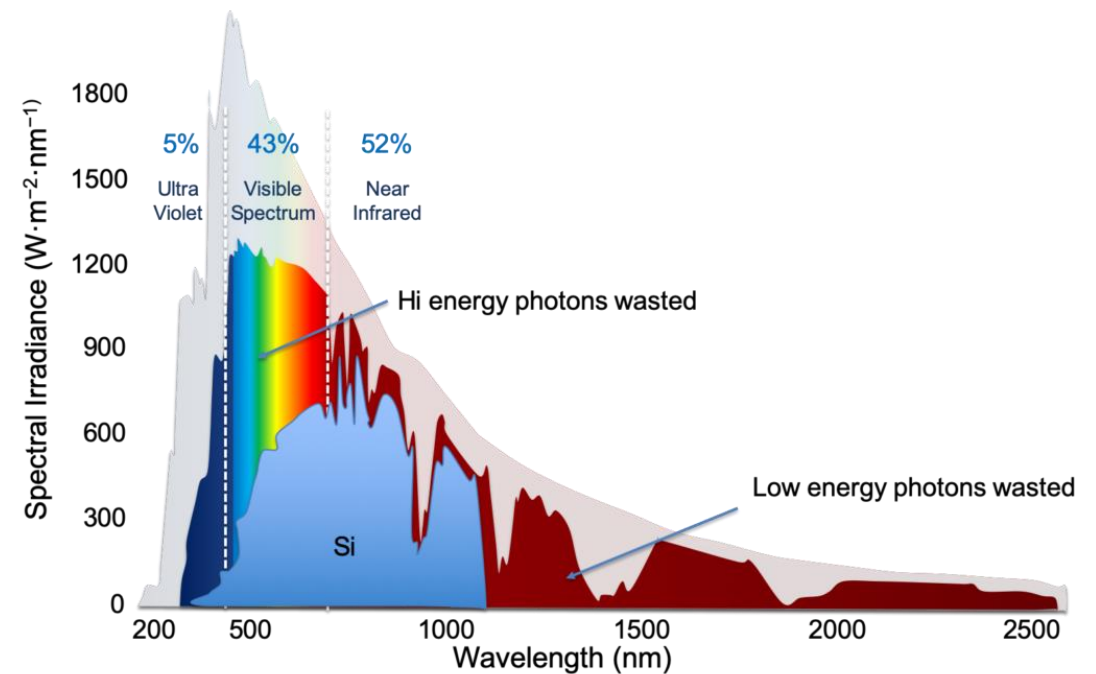


Solar energy conversion

- Photovoltaic (PV)
 - Utilize **partial solar spectrum**
 - **Low** conversion efficiency

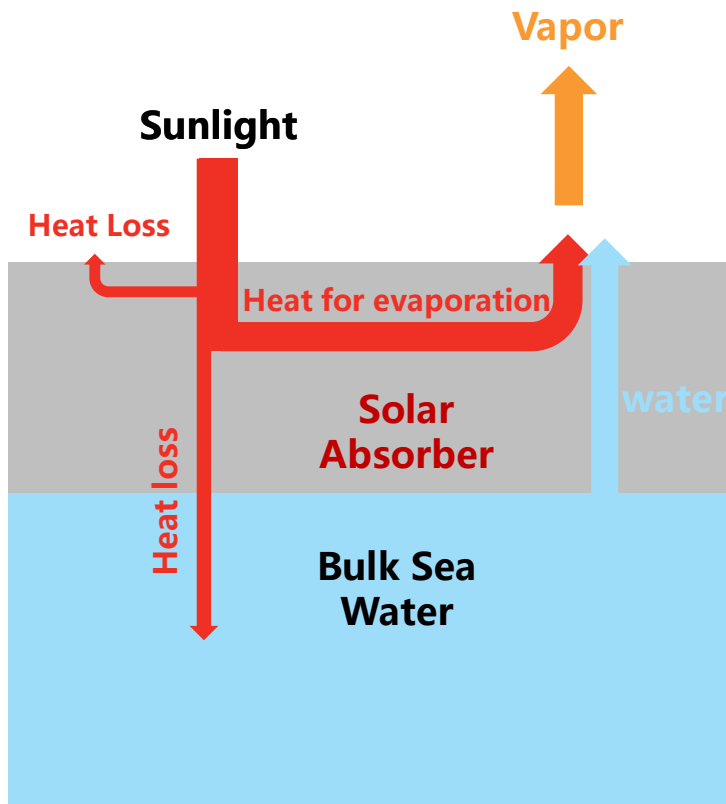


- **Solar-thermal**
 - Utilize **full solar spectrum**
 - **High** conversion efficiency



Solar-powered water evaporation

- Highly efficient utilization of solar heat for **clean water generation** by **concentrating the heat at the water/air interface** using **solar absorber**



To achieve a high energy efficiency for **solar absorber**

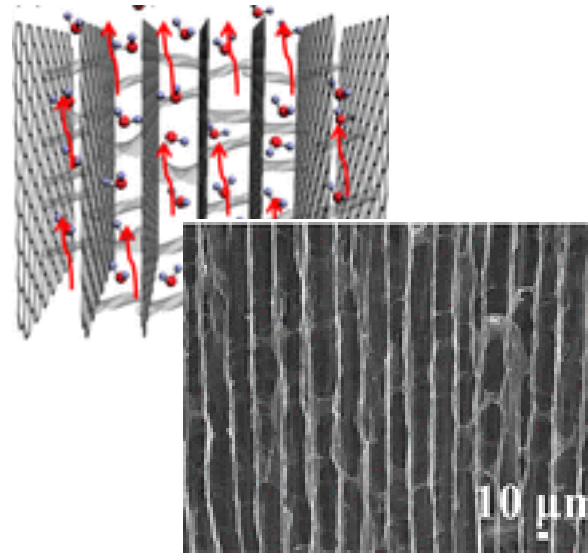
- a **high optical absorption** in the **solar wavelengths** of 0.3 to 2.5 μm to maximize the solar-to-thermal conversion
- an **excellent thermal management** to minimize the heat loss
- a proper **water management** to ensure sufficient water supply to the evaporation surface

Conventional solar absorber design

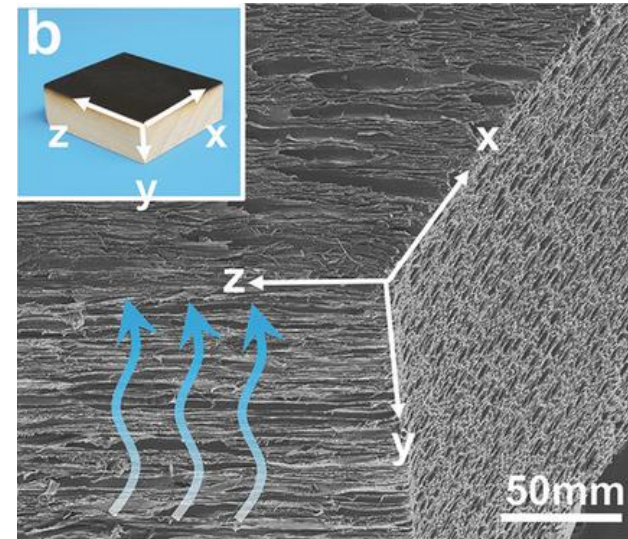
- 3D porous structure made from photothermal materials, e.g., carbon nanomaterials, plasmonic nanoparticles, MXene, etc.

Vertical pores

- Fast water transport
- Significant heat loss to bulk water



Zhang et al. *ACS Nano* 2017, 11, 5087–5093



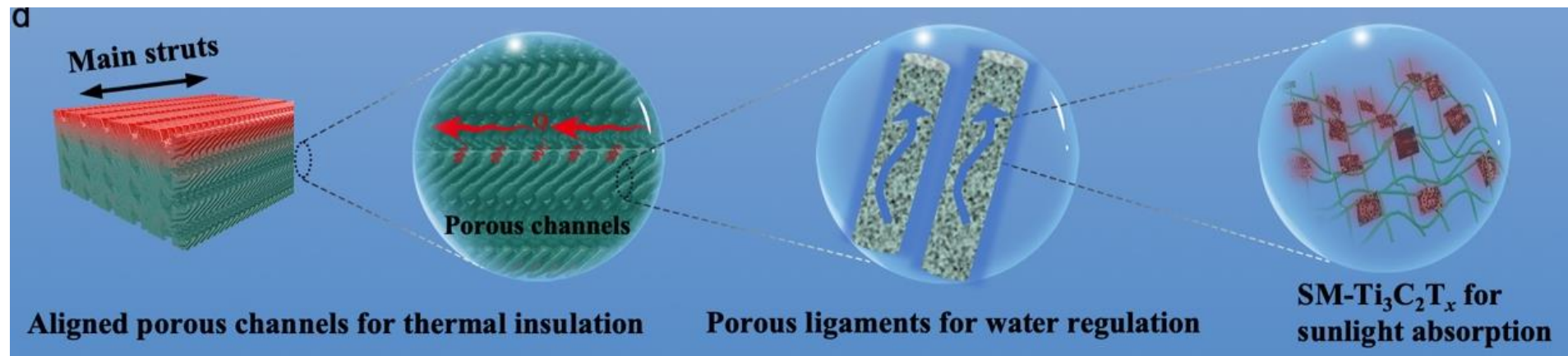
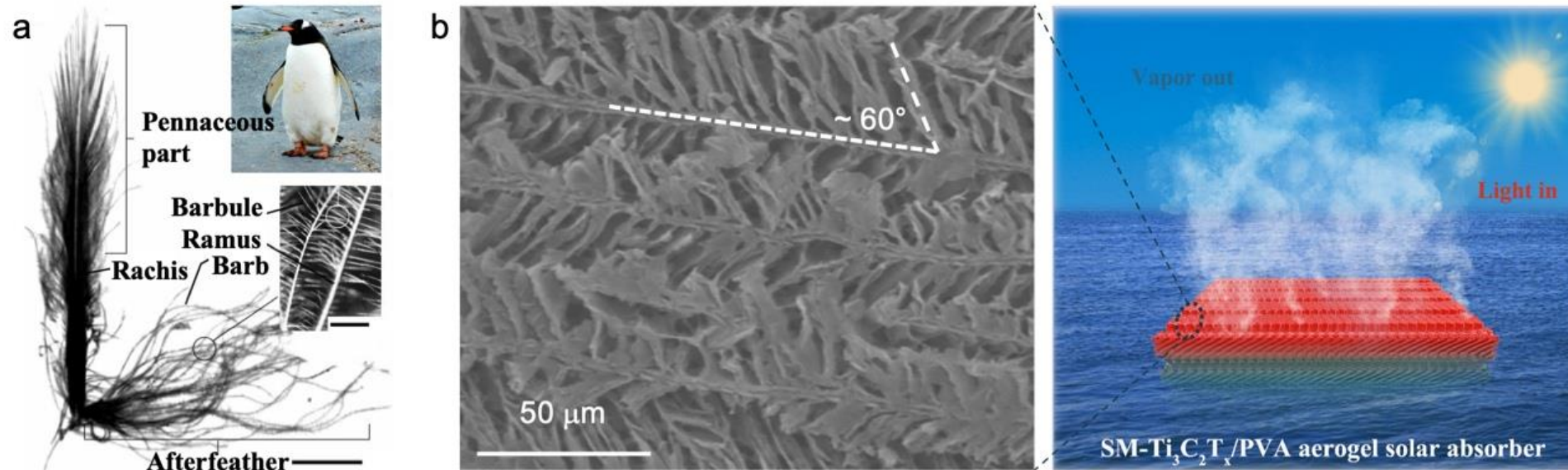
Liu et al. *Adv. Energy Mater.* 2018, 8, 1701616.

Horizontal pores

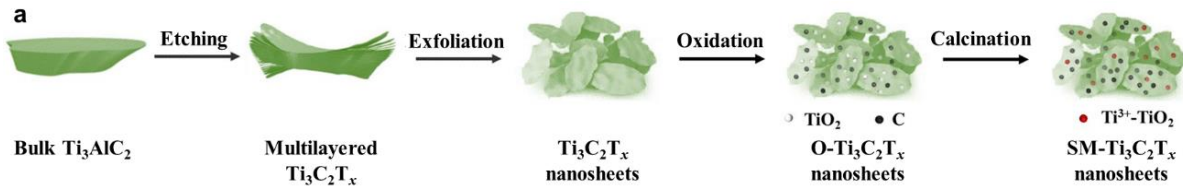
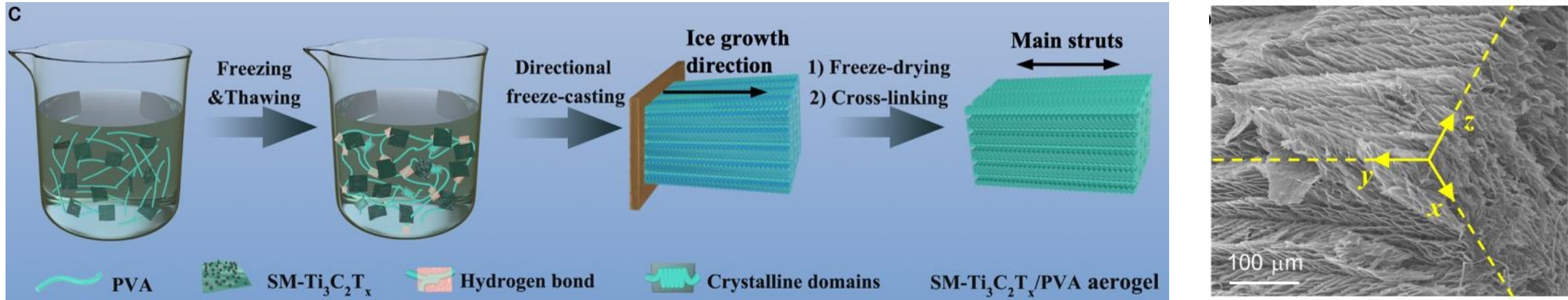
- Good thermal insulation
- Slow water transport

Simultaneously achieving fast water transport and mitigated heat loss for high energy efficiencies is highly challenging.

Biomimetic MXene/PVA aerogel for solar-powered evaporation

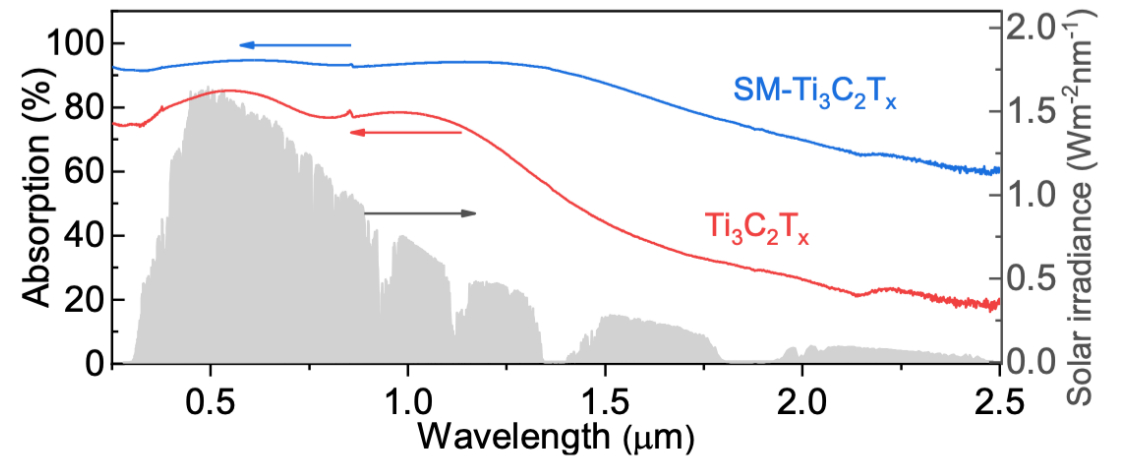


Fabrication of MXene/PVA aerogel by directional freeze-casting

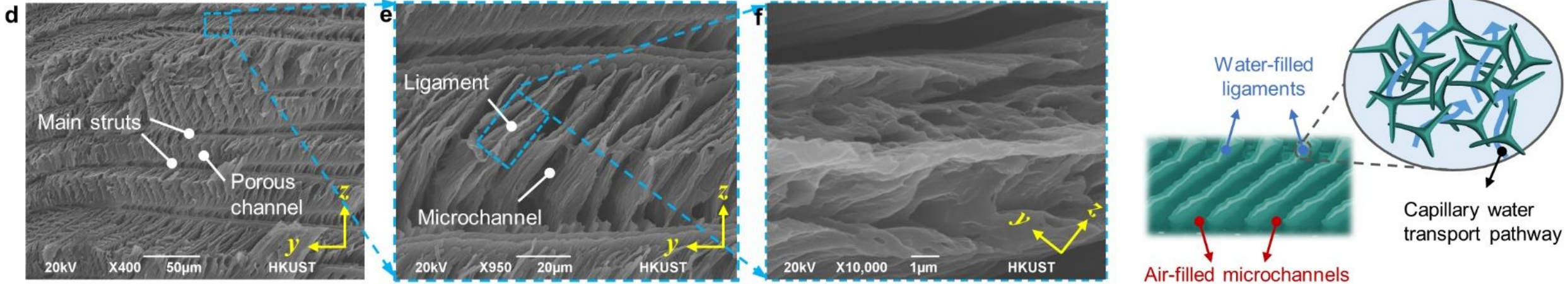


Spectrally modified Ti₃C₂T_x (SM-Ti₃C₂T_x) MXene

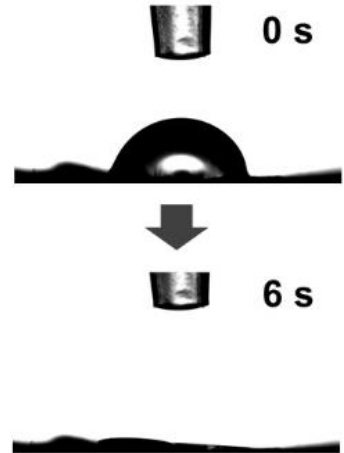
- MXene: low emissivity for low heat loss
- Introduce Ti³⁺ and TiO₂ on the surface of MXene
- Improved absorption in solar spectrum



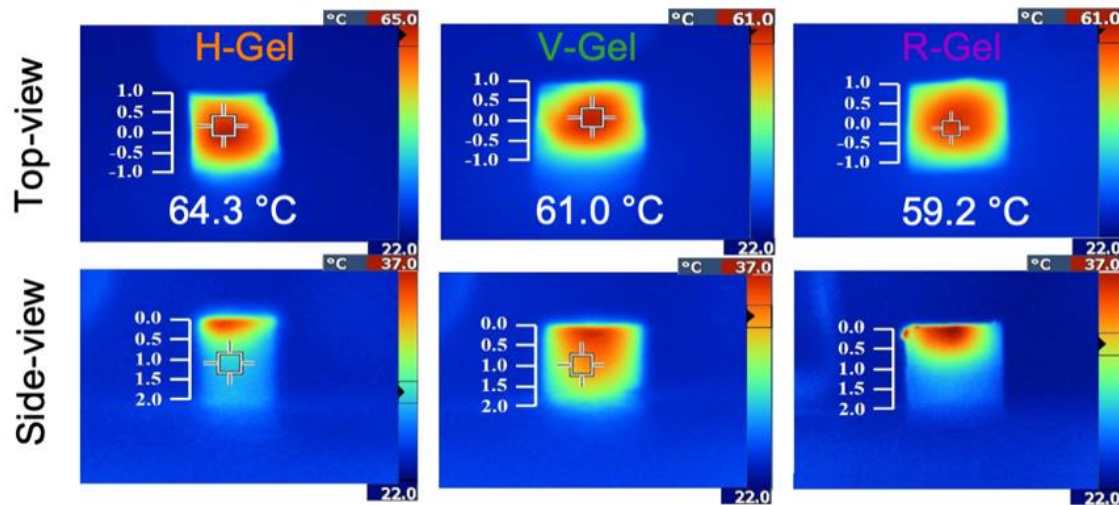
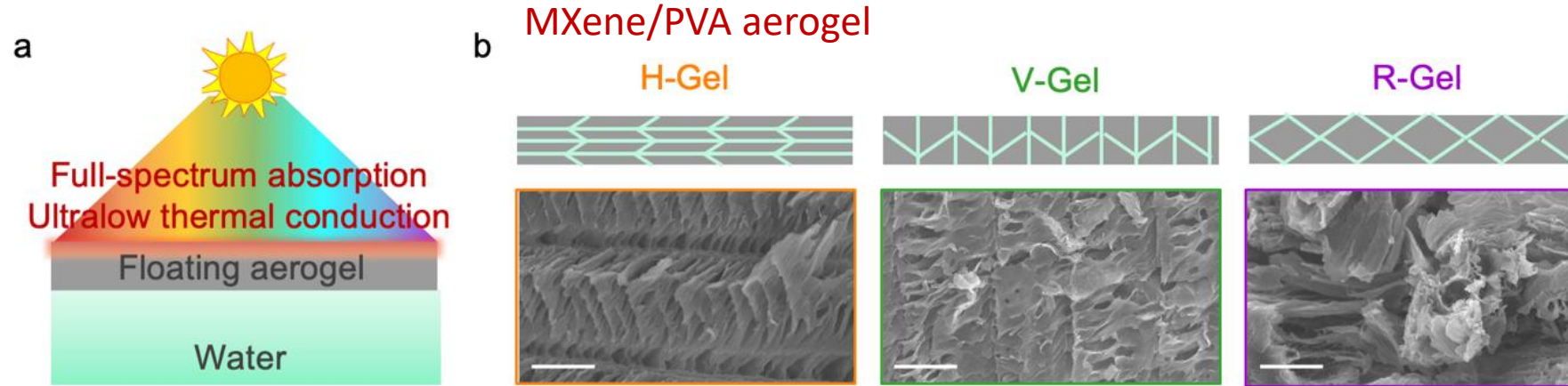
Hierarchical porous structures of MXene/PVA aerogel



- **Horizontal porous channels** ($\sim 50 \mu\text{m}$) sandwiched between main struts \rightarrow **excellent thermal insulation**
- Abundant **ligaments** formed at an angle of $\sim 60^\circ$, further dividing the porous channels into microchannels of 10 to 20 μm in the transverse direction \rightarrow **self-floating**
- Smaller **pores of less than 1 μm** inside **hydrophilic ligaments** \rightarrow **fast capillary water transport**



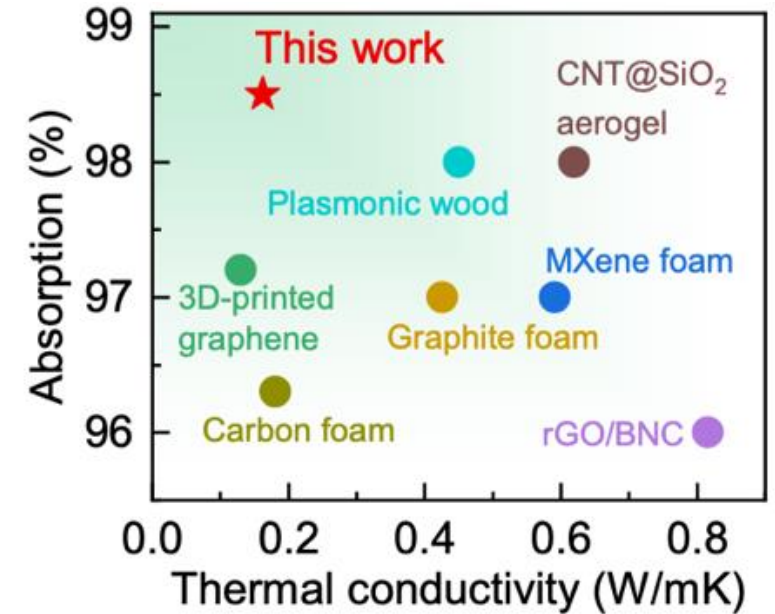
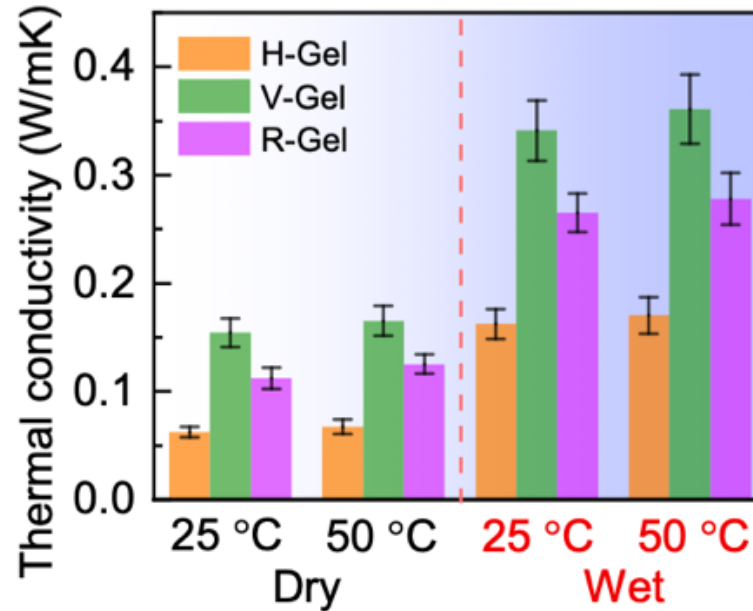
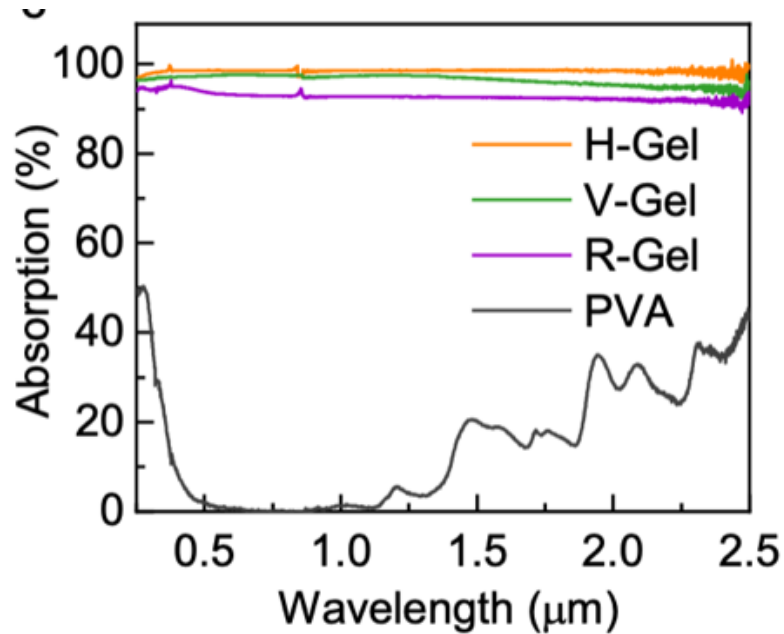
Thermal management of MXene/PVA aerogel



MXene/PVA aerogel with **horizontal pore channels (H-Gel)**

- Higher surface temperature
- Less heat loss in the thickness direction
- Better overall thermal management capability

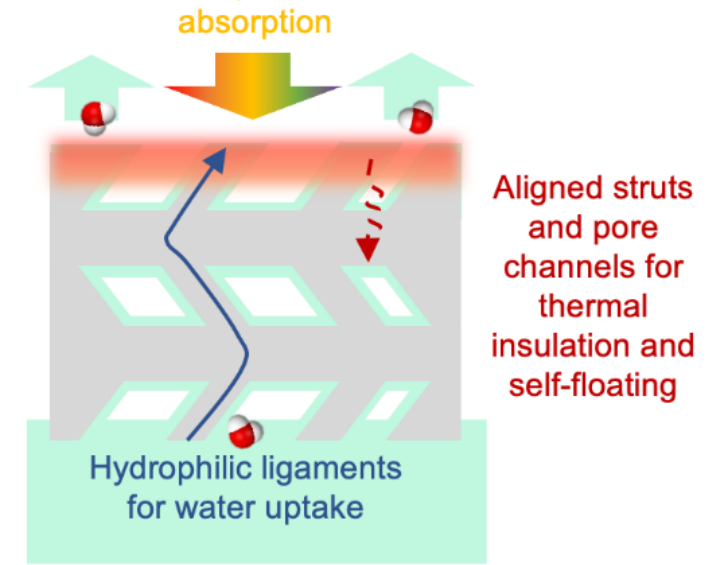
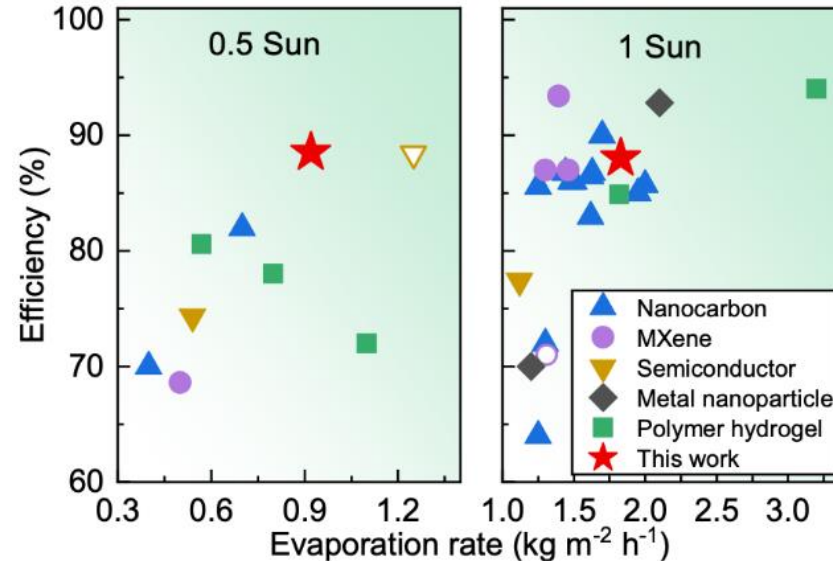
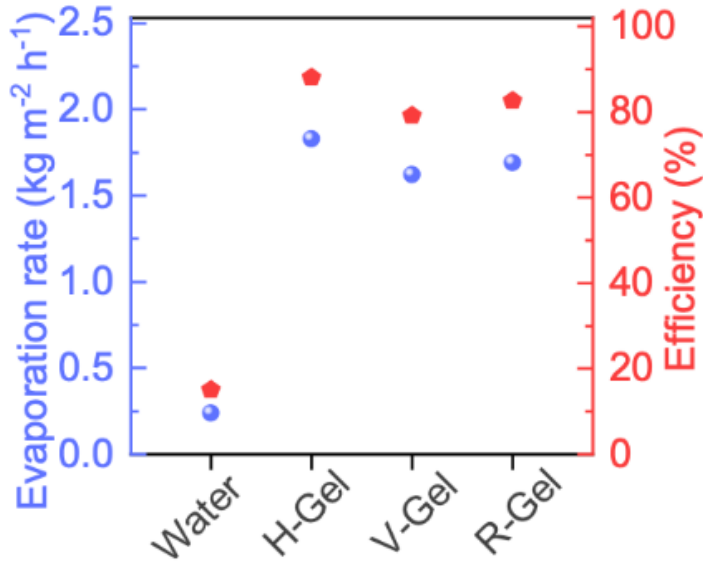
Thermal conductivity and solar absorption of MXene/PVA aerogel



MXene/PVA aerogel with **horizontal pore channels (H-Gel)**

- **98.5% absorption** of solar energy
- Low thermal conductivity of **$0.162 \text{ Wm}^{-1}\text{K}^{-1}$** even at **wet state**
- **Best combined properties** among different solar absorbers

Evaporation rate and energy efficiency of MXene/PVA aerogel



MXene/PVA aerogel with **horizontal pore channels (H-Gel)**

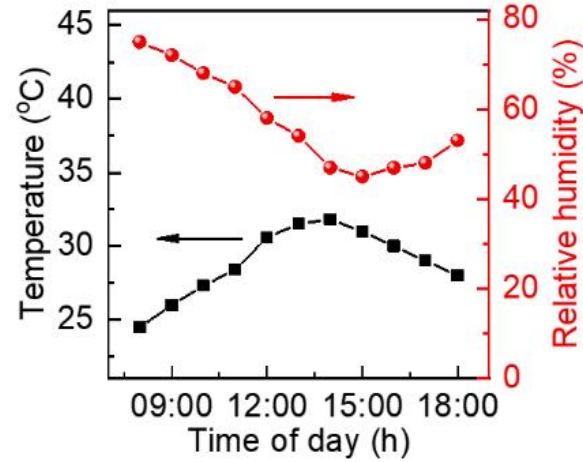
- Energy efficiency of **88 %**: higher than V-Gel and R-Gel (~80%)
- Evaporation rate of **1.83 kg m⁻² h⁻¹**: 7.9 times that of neat water
- Excellent energy efficiency and evaporation rate even **under weak solar irradiation**

Practical water desalination under natural sunlight

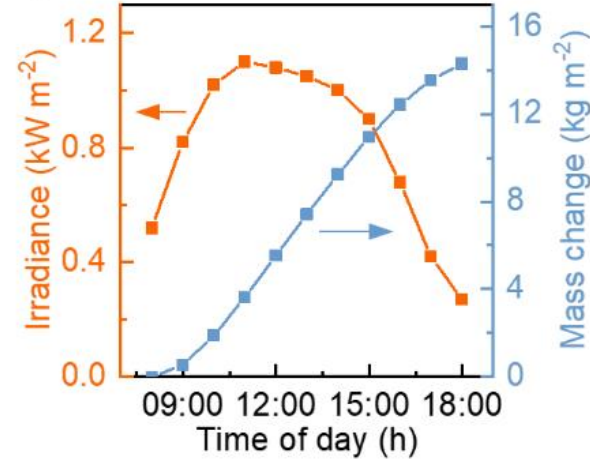
a



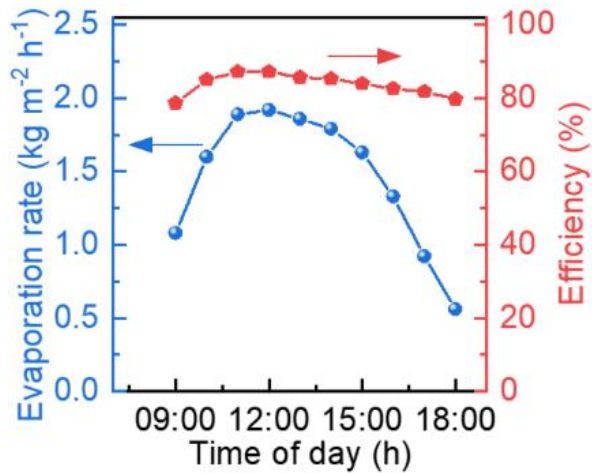
b



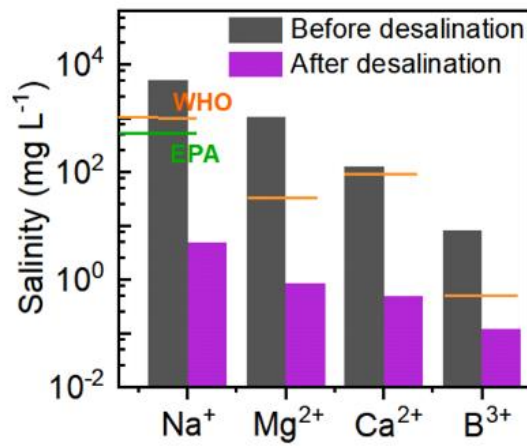
c



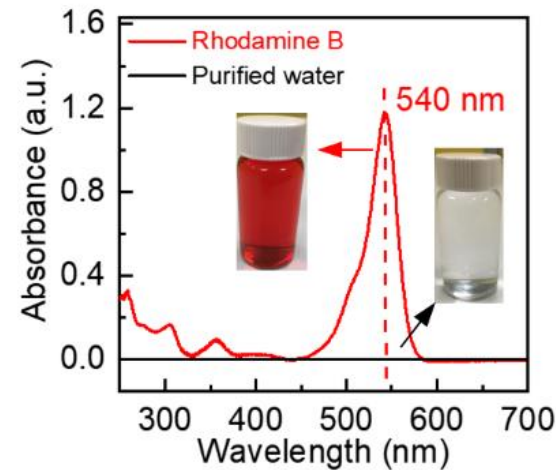
d



e



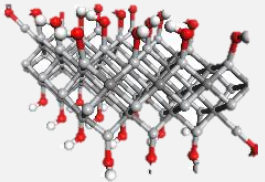
f



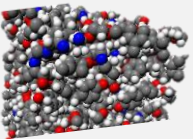
- Seawater as the source
- Average irradiance of 0.8 kW m⁻²
- Average energy efficiency of 86 %
- 14 kg of water generated after 10 hr
- Significantly reduced ion concentrations safe for drinking

Conclusions and outlook

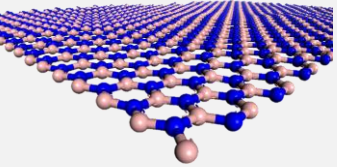
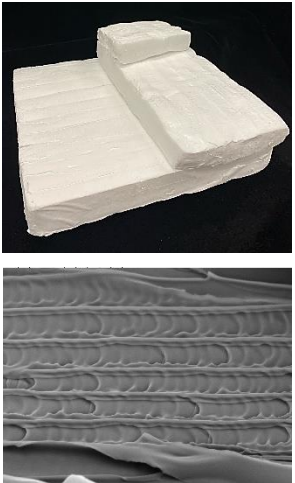
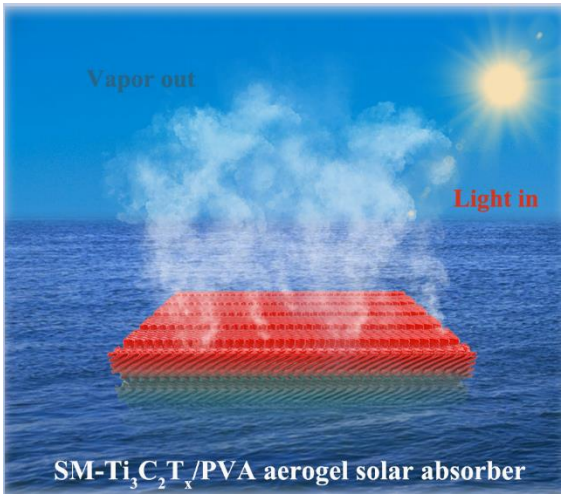
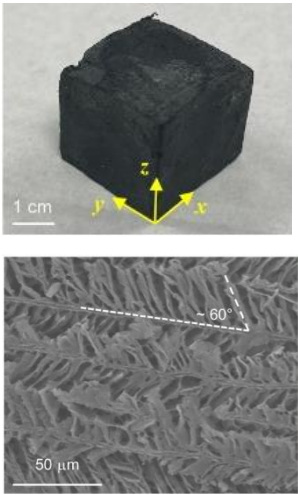
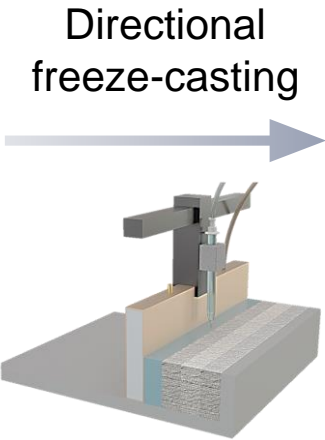
MXene



Polymer matrix



Boron nitride nanosheets (BNNS)

Energy-efficient heating

- Thermally insulating
- Solar absorptive

Energy-efficient cooling

- Thermally insulating
- Solar reflective