2021 Edith and Peter O'Donnell Awards

Multifunctional Hydrogels as An Emerging Platform for Energy and Water Sustainability

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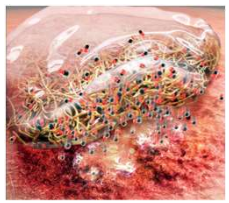
Hydrogel — A Unique Class of Functional Materials

"Jelly-like" solids with elastic nature, capable of retaining large amounts of water and maintaining hierarchical structures.

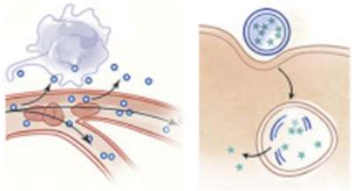
Baby diapers

Contact lenses

Wound healing



Drug delivery



Air freshers

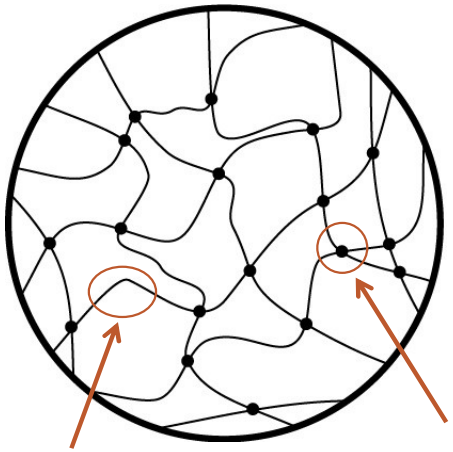
Jiggly desserts

Tissue engineering

Hydrogels in daily life

Hydrogels in biology/medicine

Crosslinked networks

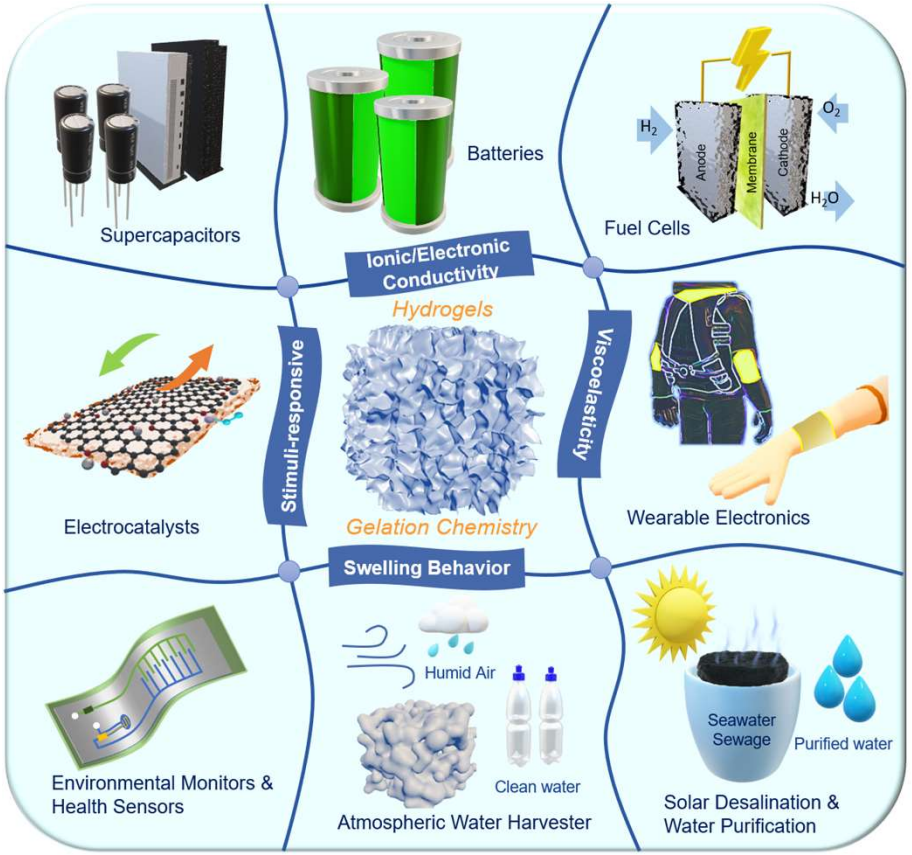


Building blocks:
Polymer, Carbon,
Inorganic compounds…

Crosslinking point:
Chemical bonds or
Physical interactions

Peppas and Langer, ***Advanced Materials*** 2006.

Hydrogel — Tunable Physiochemical Properties



Synthetically tunable systems

Monomer/polymer Crosslinking

Polymer-water interaction

Functional groups Additive materials

Hydrogels as an Emerging Material Platform for Water-Energy Technologies

Guo, Bae, Yu, ***Chemical Reviews*** 2020.

From Synthesis/Self-Assembly to Energy-Water Technologies

Hydrogels

Organic: Monomers (aniline, pyrrole..) + Crosslinkers (CuPcTs, PA..)

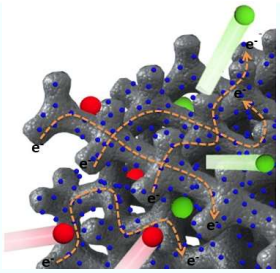
Graphene: Graphene (Oxide) + Crosslinkers (ions, biomolecules..)

Inorganic: Metal centers + Ligands (-CN, -OH.)

Gelation ↓ Self-assembly

Networks

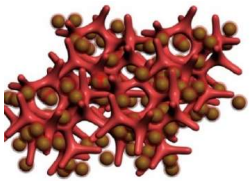
Chemical functionalization ↓



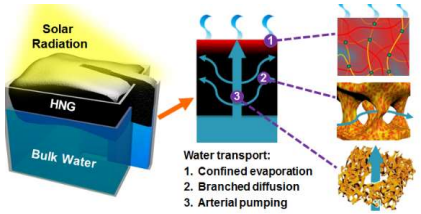
Hydrogel-derived frameworks

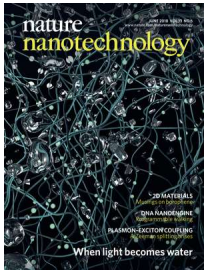
- Macro/mesopores for ion diffusion
- High conductivity for charge transfer
- Controlled dopants
- Self-supporting structure

Energy Storage/Conversion



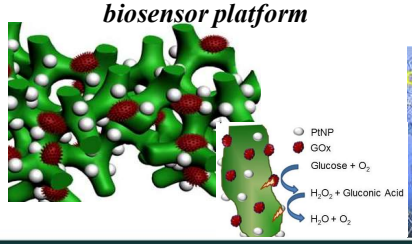
Solar Water Desalination/Harvesting



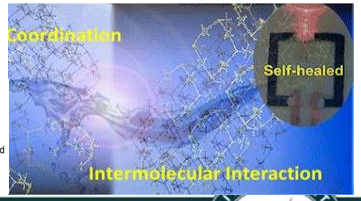


Responsive/Adaptive Materials

biosensor platform

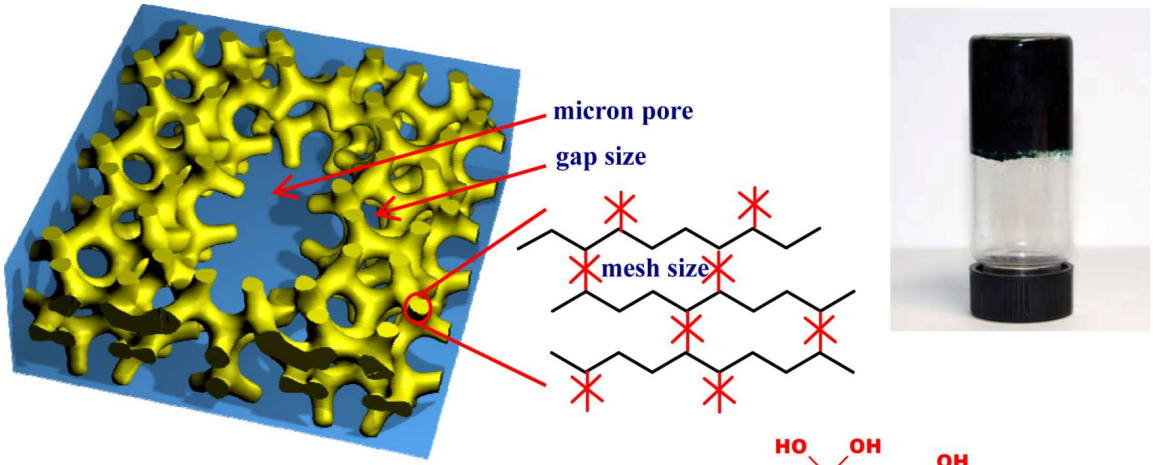


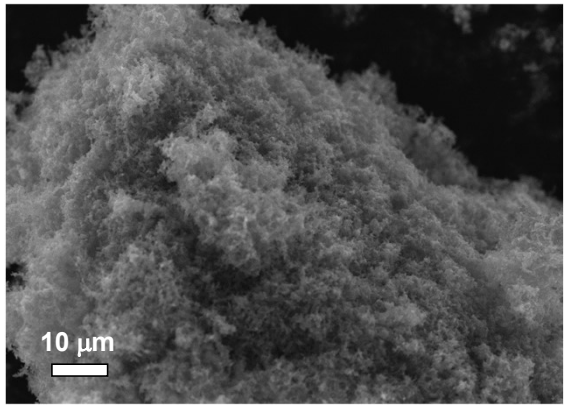
self-healing supergel

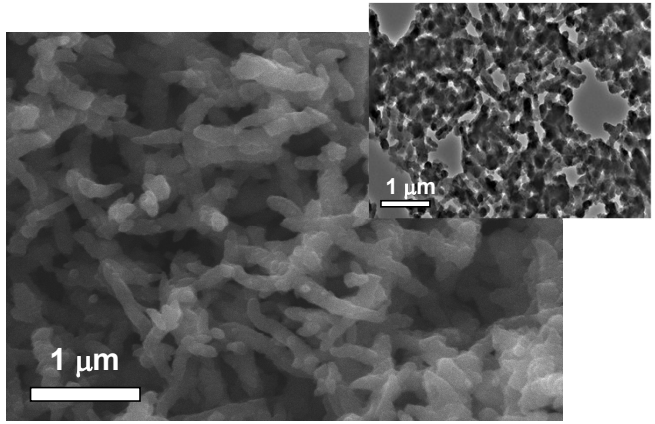


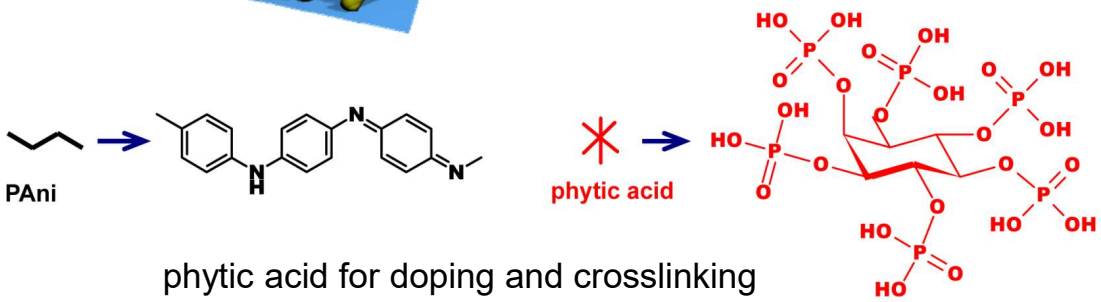
Hierarchically Porous Nanostructured Hydrogels

nanostructured conducting polymer hydrogels (nCPHs)





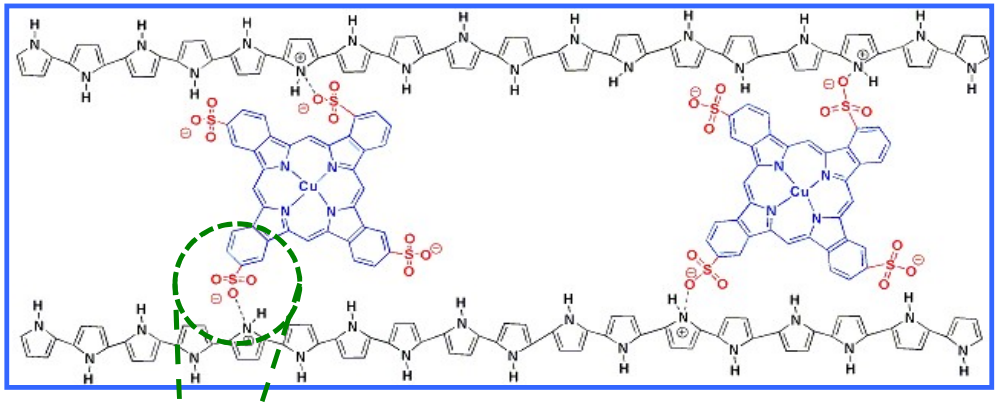


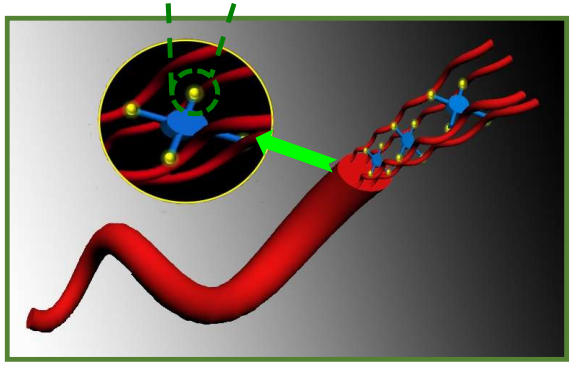


phytic acid for doping and crosslinking

Pan, Yu, Bao, ***PNAS,*** 2012.

Dopant-Enabled Supramolecular Synthesis





Ppy doped with CuPcTs

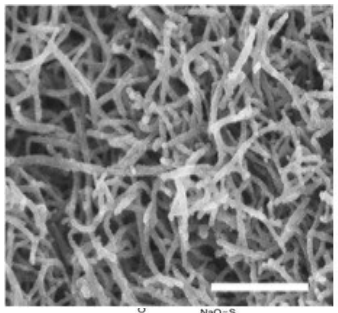
→ **Polypyrrole**

→ **CuPcTs**

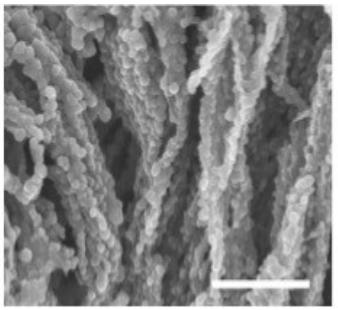
CuPcTs:
copper phthalocyanine-3,4',4'',4'''-tetrasulfonic

Tetra-functional groups

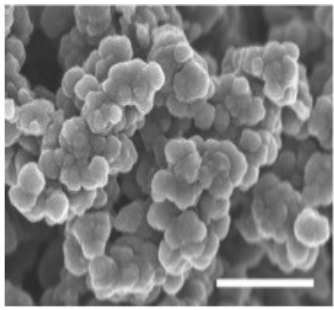
1D nanowire network



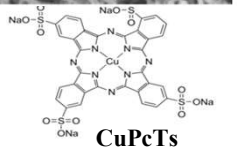
1D NP-assembled 'necklace'



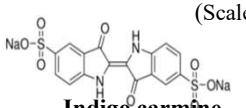
3D nanoparticle 'clustering'



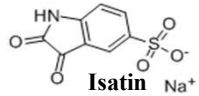
(Scale bar: 1μm)



CuPcTs



Indigo carmine



Isatin

nano-confinement through molecular design

Table 1. Measured Conductivities of Different PPy Samples with Different Dopants

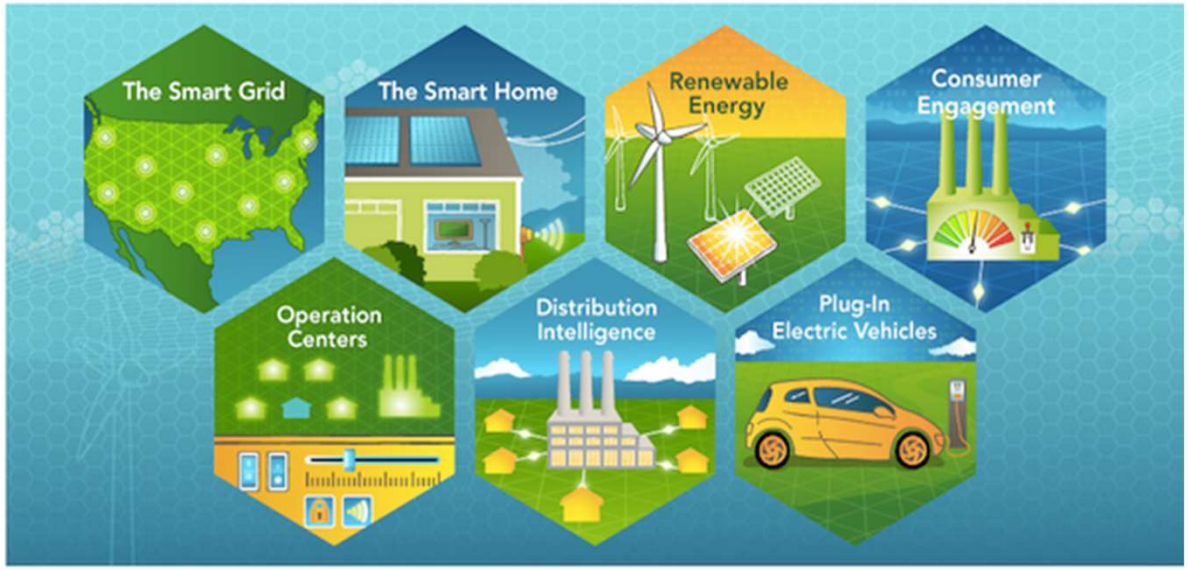
samples	PPy–CuPcTs	PPy–indigo	PPy–isatin	pristine PPy
conductivity (S/cm)	7.8	0.4	0.06	0.07

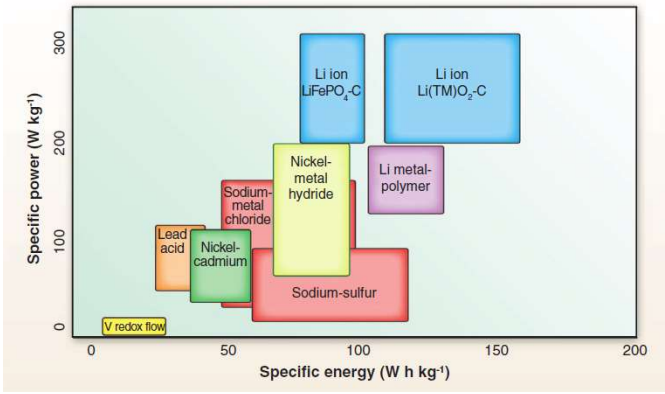
Enhanced conductivity

Wang, Shi, Yu, ***Nano Letters,*** 2015.

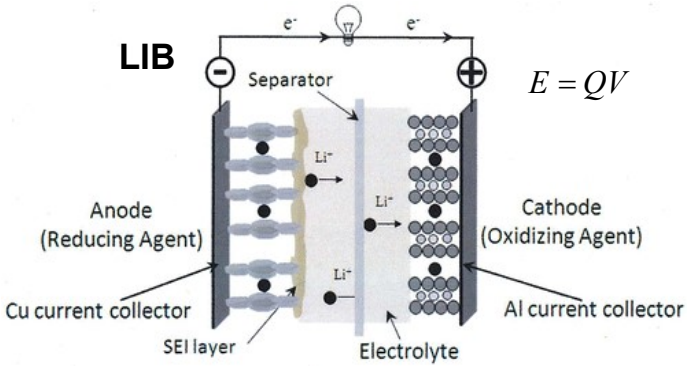
Energy Storage Landscape and Technologies

Electric energy storage:
A key component for future energy economy





Dunn, Tarascon, ***Science,*** 2011.

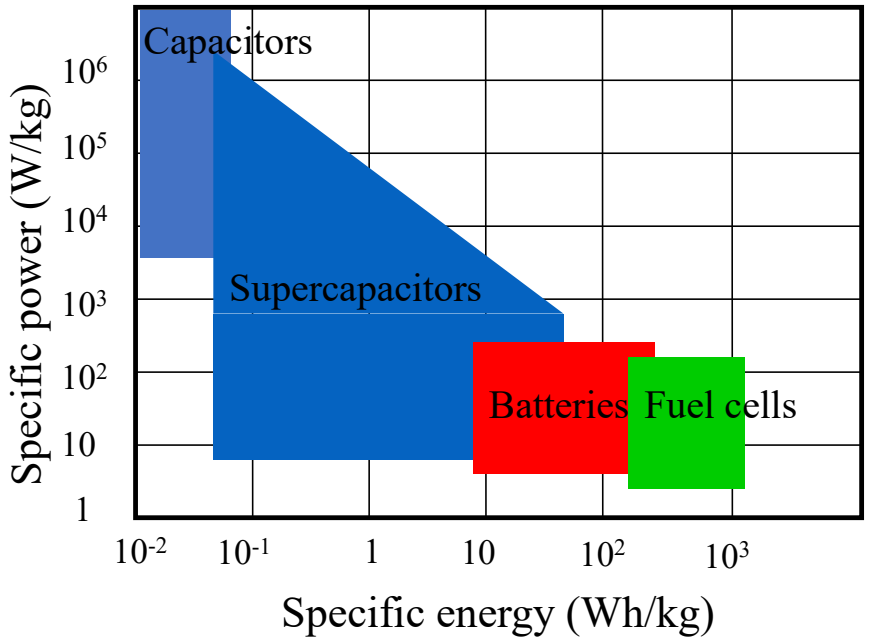


Goodenough, ***Acc. Chem. Res.*** 2013.

Advancing Energy Storage Technologies

Supercapacitor

Li-ion Battery

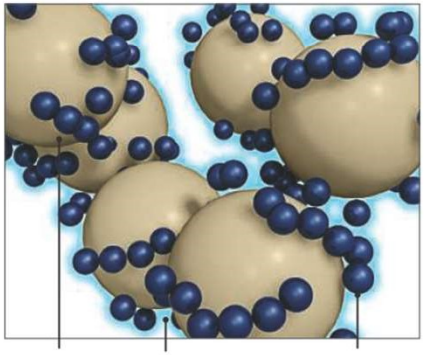


Key parameters:

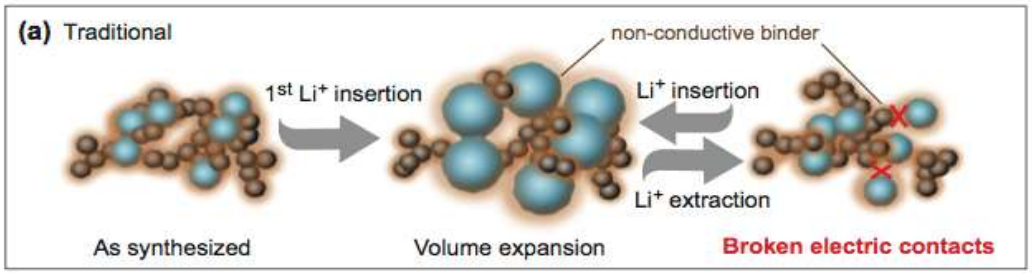
- Energy density (per weight/volume)
- Power density
- Cycle life
- Safety and Cost

Multifunctional Hydrogels for Energy Storage

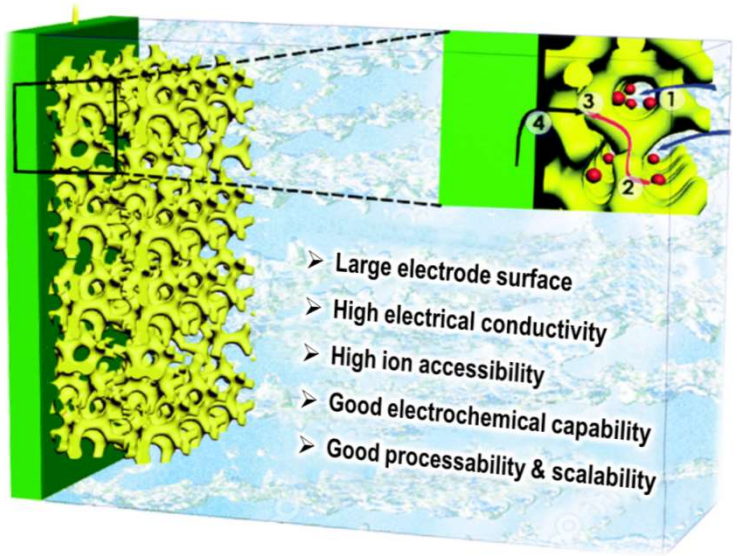
traditional electrodes in LIBs



- **Electrons are conducted via chains of particles through the composite**
- **A randomly distributed mixture of conductive phases**
- **Bottlenecks and poor contacts may impede effective access to parts of the battery**

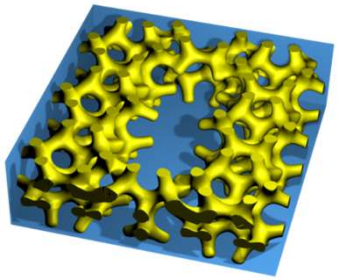


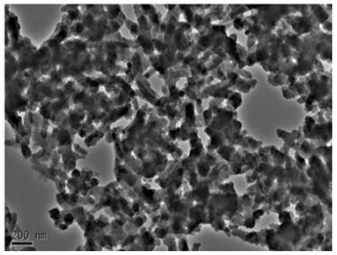
Dudney, ***Science*** 149 (2015)



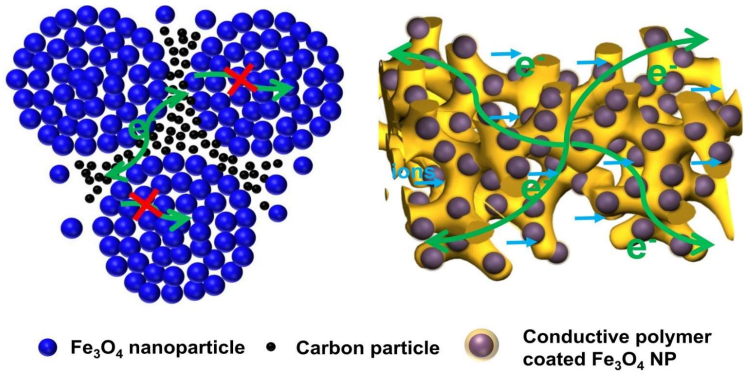
Shi, Peng, Yu, ***Chem. Soc. Rev.*** 2015;
Bonaccorso, Colombo, Yu, ***Science*** 2015.

Tunable 3D nCPHs as Framework Electrodes



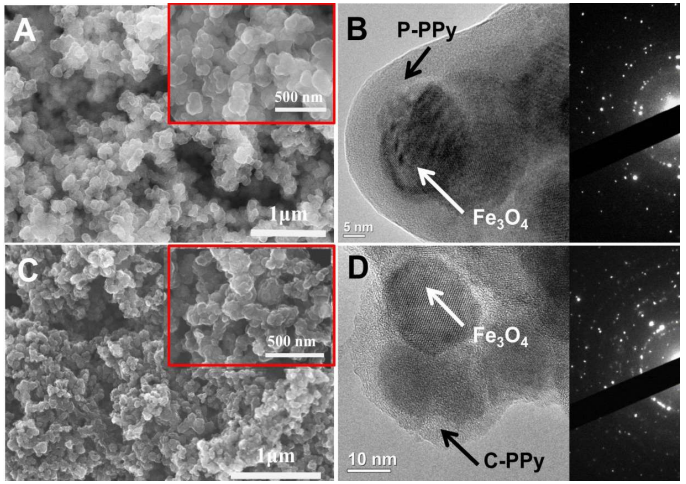


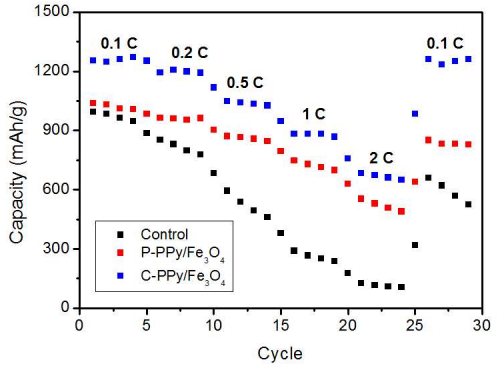
‘bi-functional binder’



Key Features:

- **CPH constructs a 3D conductive network in the electrodes;**
- **Porous structure enables fast mass/charge transport;**
- **Uniform polymer coating on the particles.**

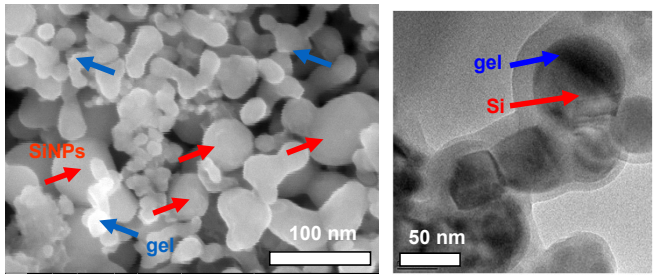


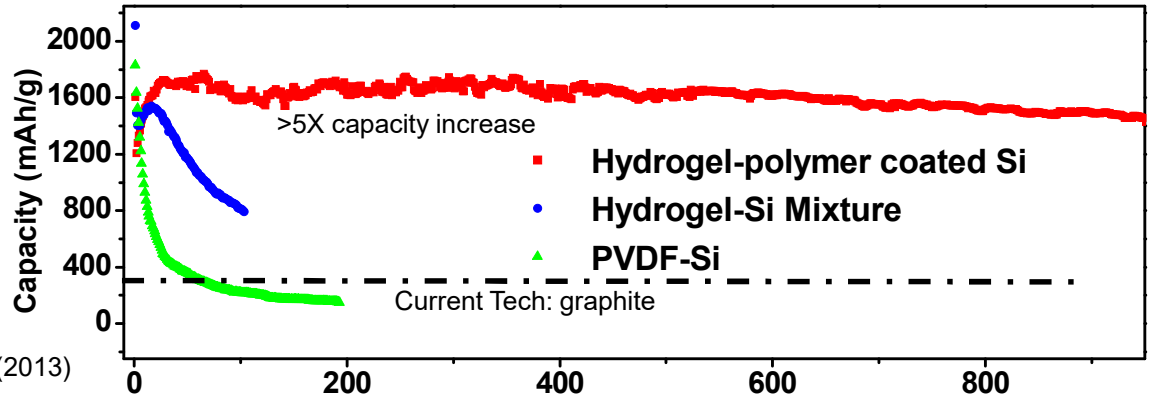


Shi, Takeuchi, Yu, ***Adv. Mater.*** 3922 (2017)

A Universal Strategy for High-Capacity Battery Electrodes

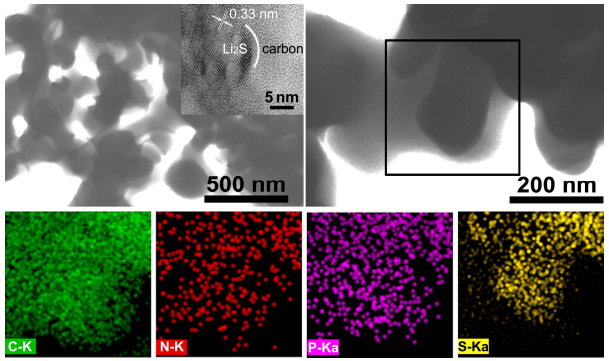
Si-Gel system

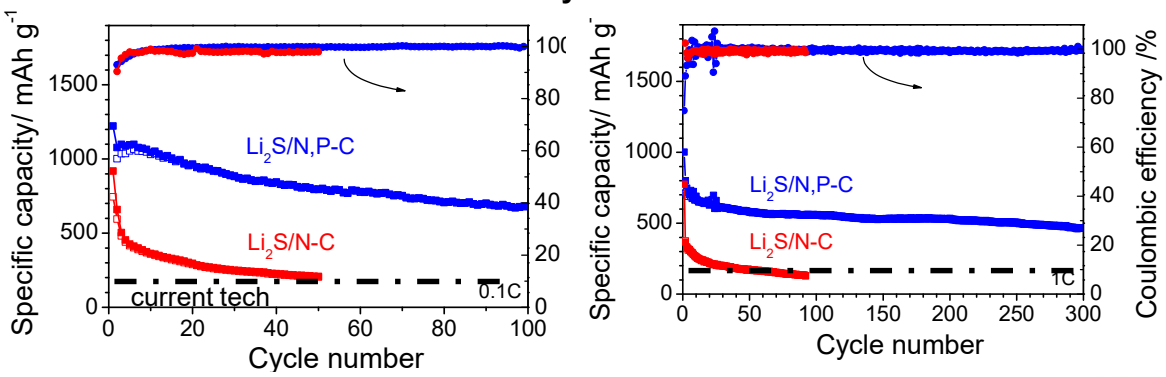




Nature Commun. 1973 (2013)

Sulfur-Gel system

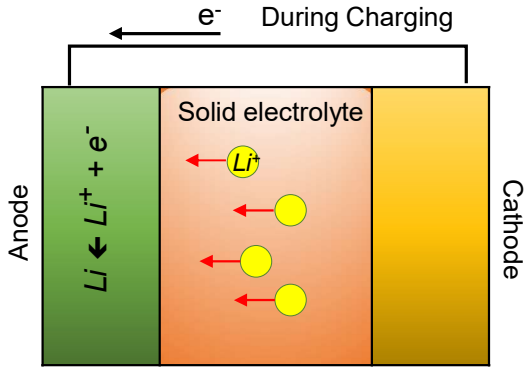




Adv. Energy Mater. 2876 (2017)

nCPH-Derived Electrolytes for Solid-State Battery

❖ **Solid state electrolyte (SSE)**

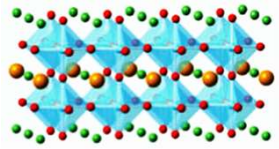


- Removing flammable liquid electrolytes
- High cycling stability ➔ solid-solid interface
- Suppressing dendrite growth by solid electrolyte

ISE: Inorganic solid electrolyte

Inorganic material, fixed lattice

Lithium lanthanum titanate
$Li_{0.33}La_{0.56}TiO_3$

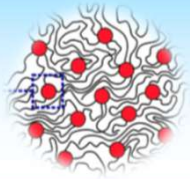


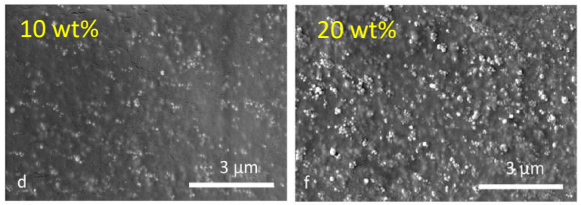
Versus

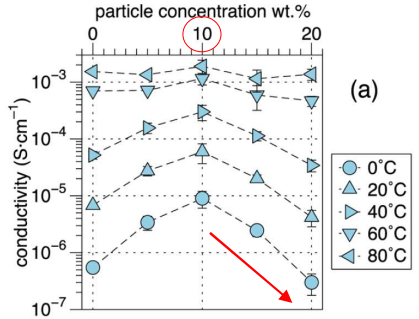
CPE: Composite polymer electrolyte

Composite of Inorganic filler + Polymer

SiO_2 nanoparticles
in PEO matrix







J. Phys. Chem. C 2017, 121, 2563

- Agglomeration at high concentration
- Deterioration of ionic conductivity

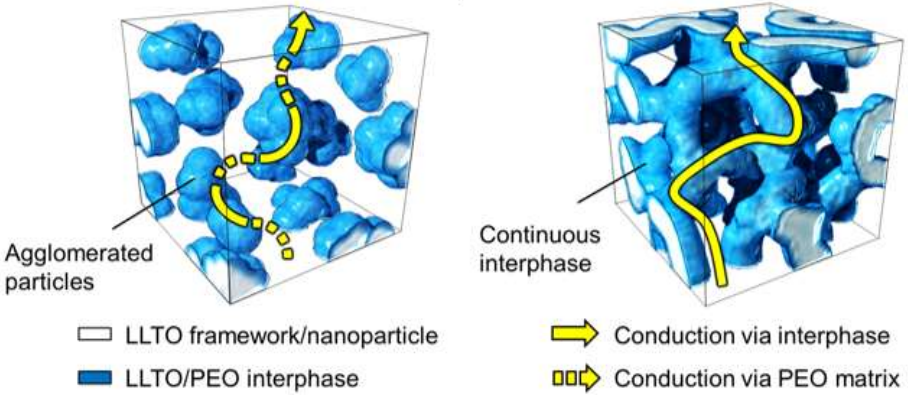
- **Challenges in Solid State Battery**

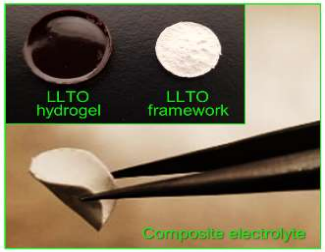
- Li metal ➔ dendrite suppression vs delamination
- Poor rate capability ➔ high internal resistance at the interfaces
- Electrochemical instability at the electrolyte/electrode interface

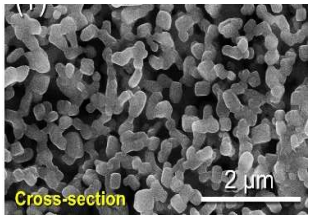
nCPH-Derived Composite Polymer Electrolytes

High weight ratio of ceramic fillers & maintaining percolation network

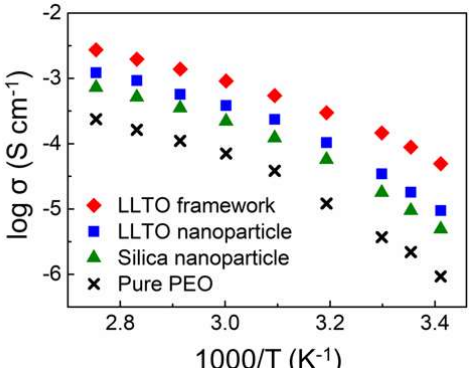
➔ Enhanced conductivity & electrochemical stability



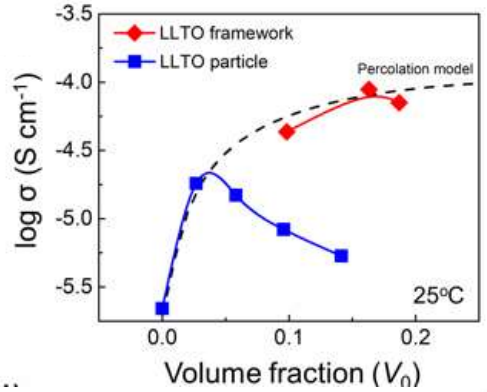




Conductivity with different types fillers



LLTO framework percolation model

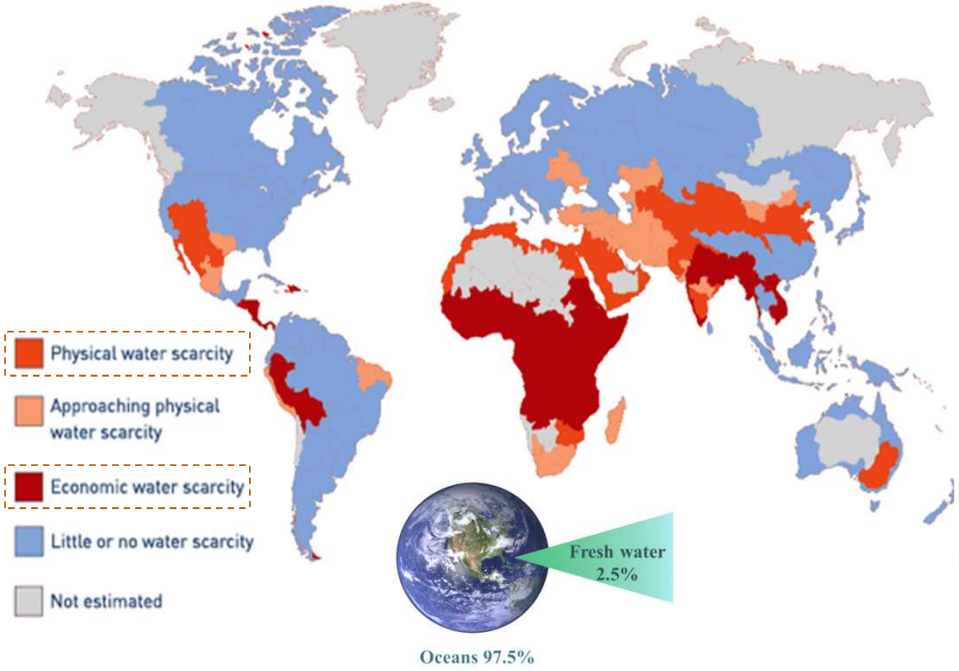


Bae, Goodenough, Yu, ***Angew. Chem. Int. Ed.*** 2096 (2018)

Global Clean Water Scarcity

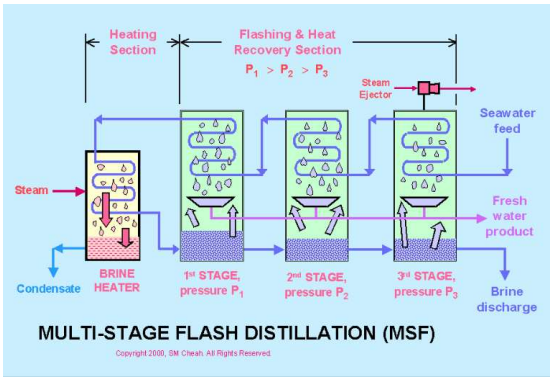
3 Billion

Living in areas of high water stress



WWAP, UN.org, Iwmi.cgiar.org,

Major Industrial Desalination Technologies

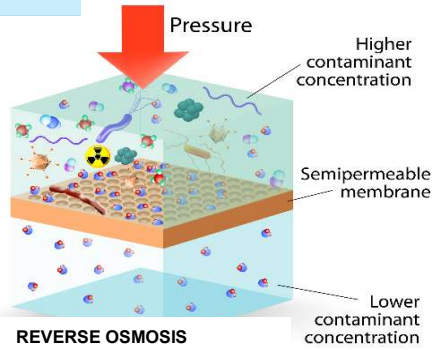


Thermal-based

- High energy consumption
- Large, centralized infrastructures

Membrane-based

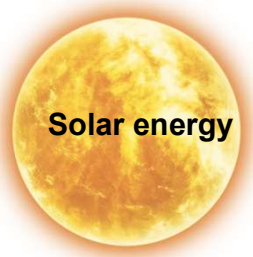
- Require high pressure
- High cost of membrane (prone to fouling)



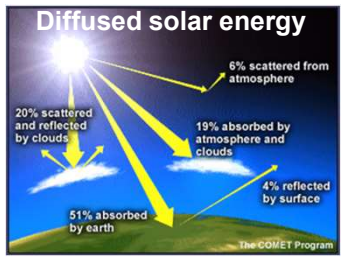
Mezher, *Desalination* 2011, 266, 263; Service, *Science* 2006, 313, 1088.

Solar-Powered Water Purification

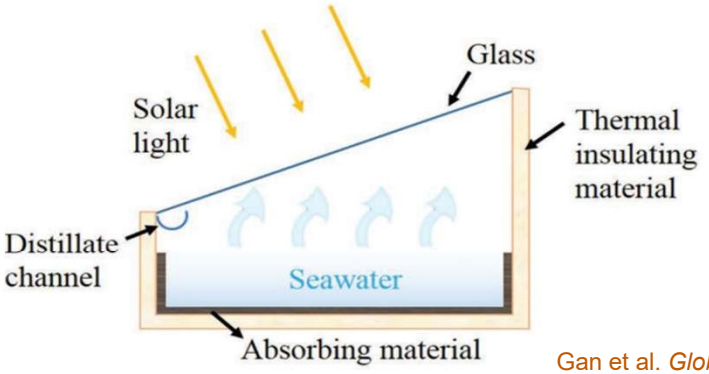
An electricity-independent path to mitigate water scarcity using only sunlight



Optical loss



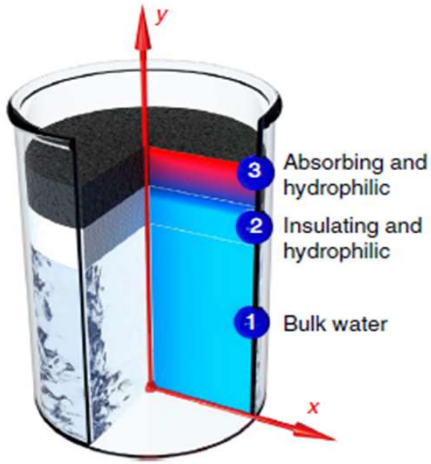
Conventional Solar Still



Heat loss

Gan et al. *Global Challenges* 2017, 1600003.

Interfacial Evaporation

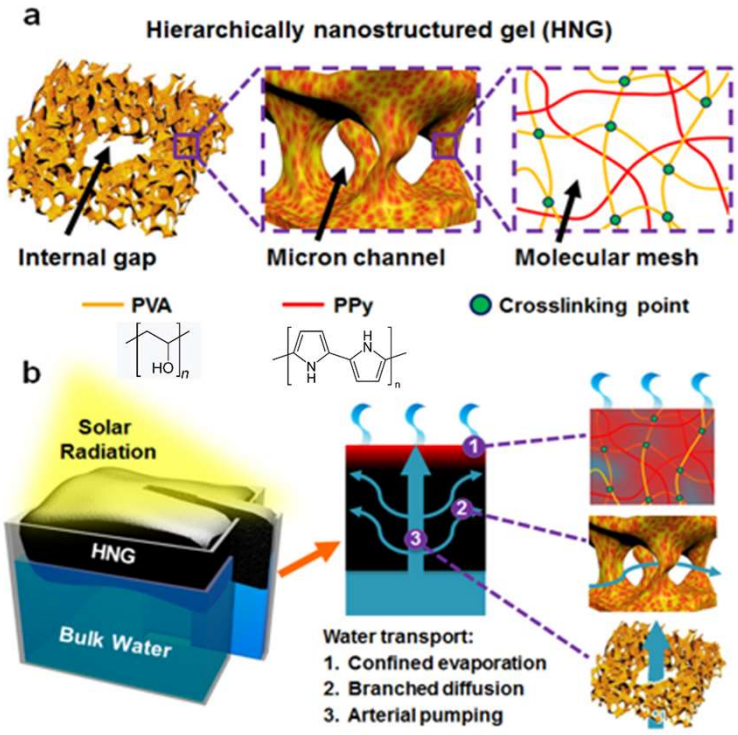


- High solar absorption
- Heat localization
- Fast water transport

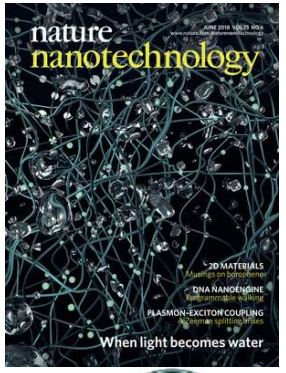
Chen et al. *Nature Commun.* 2014, 4449.

Hydrogel-based Solar Vapor Generator

An efficient way of harvesting solar energy for purification of polluted or saline water.

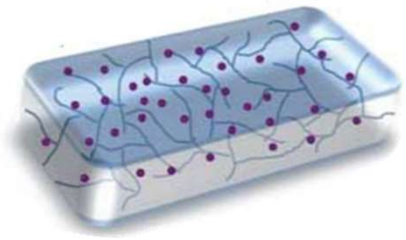


- **Confined evaporation**
  Solar heat used for evaporation can be localized by PVA gel at the water-air interface→reduce the energy loss of bulk water at the bottom
- **Branched diffusion and arterial pumping**
  Micron channels and internal gaps of PVA gel can generate capillary force to rapidly replenished molecule meshes from bulk water below.
- **Polymer gel network reduce latent evaporation enthalpy of water**

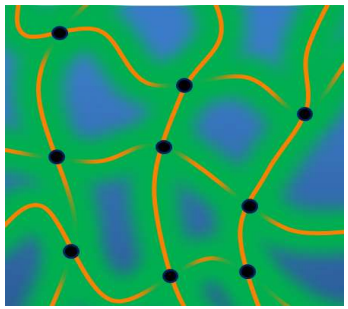


Zhao, Zhou, Yu, ***Nature Nanotech.*** 489 (2018).

Unique Hydrogel-Water System



Hydrogel: 3D crosslinked polymeric networks saturated with water.



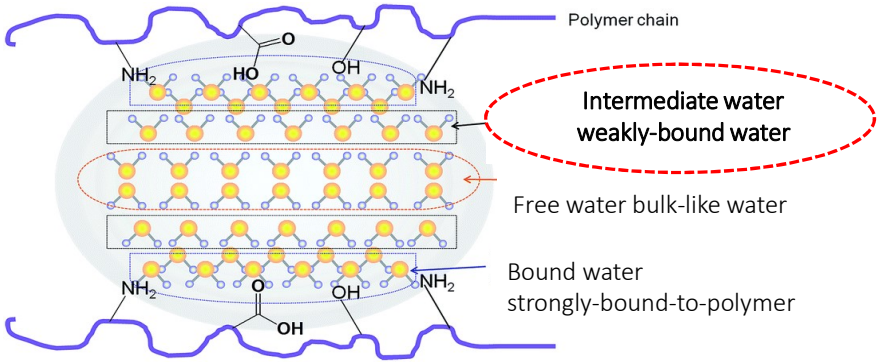
Free water

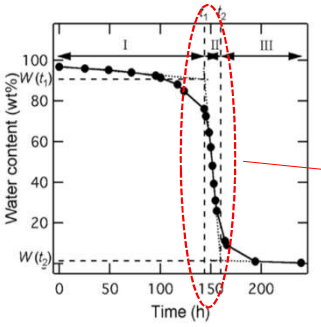
Intermediate water

Bound water

J. Chem. Phys. 2014, 044909;
Acc. Chem. Res. 2014, 2846.

Schematic of polymer chains affinity to water molecules





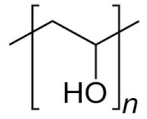
Dehydration process of PVA hydrogel

Evaporation stage of water types

(1) Free water

(2) Intermediate water

(3) Bound water

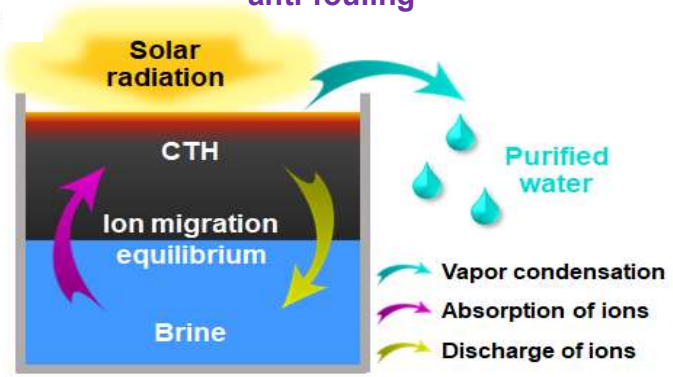


Faster evaporation rate

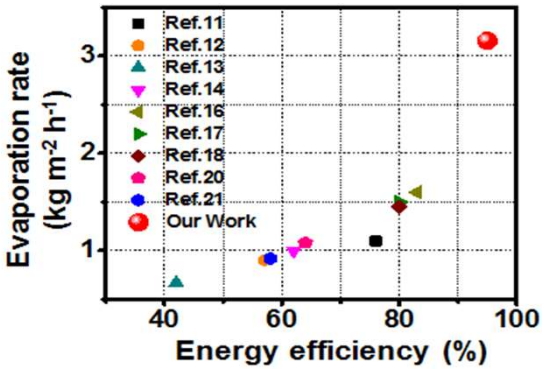
J. Mol. Struct, 2008, 282.

Features of Hydrogel-based SVG

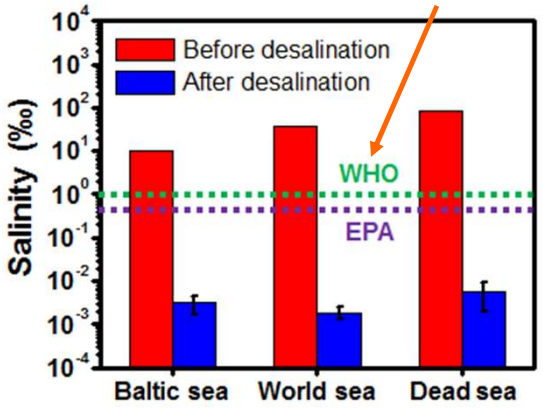
anti-fouling



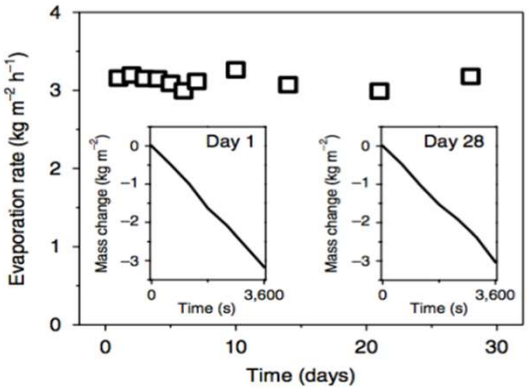
record high solar evaporation rate



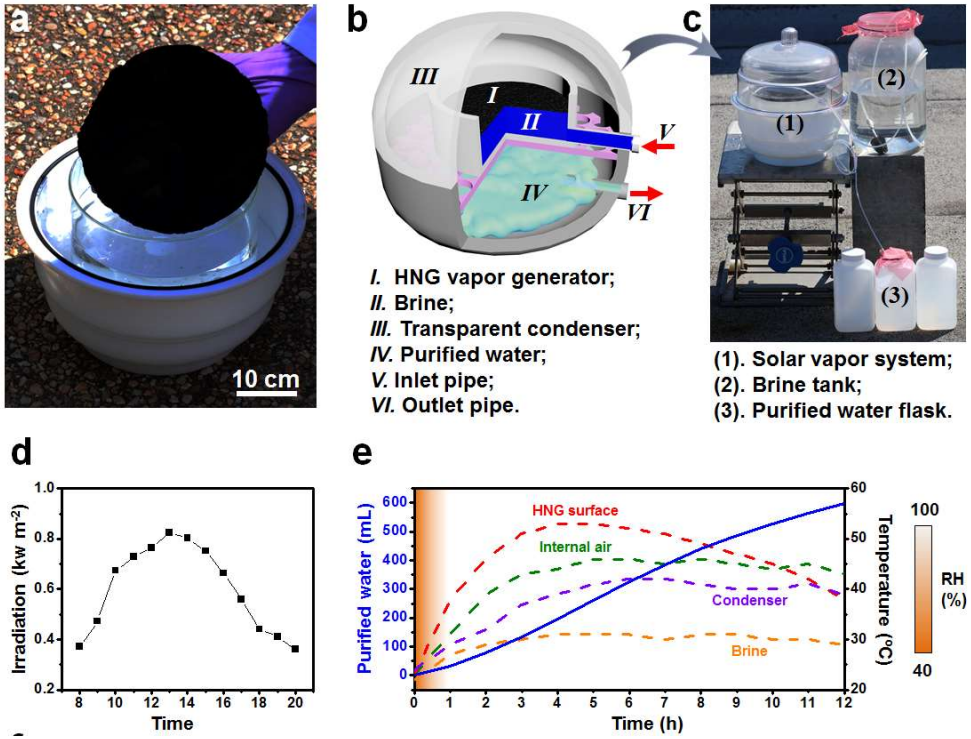
Salinity criterion of drinkable water

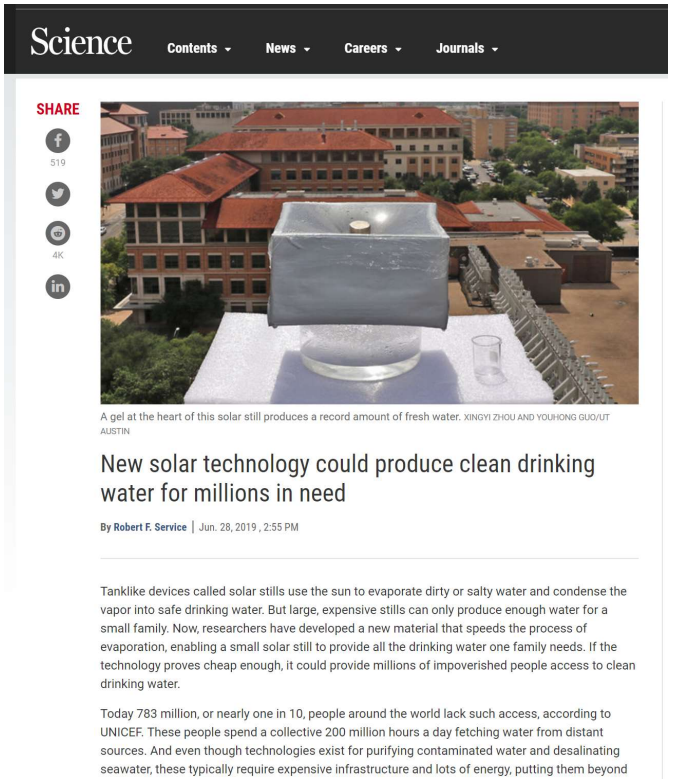


Stable SVG for continuous operation



Solar Water Purification under Natural Sunlight




Science Contents News Careers Journals

SHARE

A gel at the heart of this solar still produces a record amount of fresh water. XINGYI ZHOU AND YOUHONG GUO/UT AUSTIN

New solar technology could produce clean drinking water for millions in need

By Robert F. Service | Jun. 28, 2019 , 2:55 PM

Tanklike devices called solar stills use the sun to evaporate dirty or salty water and condense the vapor into safe drinking water. But large, expensive stills can only produce enough water for a small family. Now, researchers have developed a new material that speeds the process of evaporation, enabling a small solar still to provide all the drinking water one family needs. If the technology proves cheap enough, it could provide millions of impoverished people access to clean drinking water.

Today 783 million, or nearly one in 10, people around the world lack such access, according to UNICEF. These people spend a collective 200 million hours a day fetching water from distant sources. And even though technologies exist for purifying contaminated water and desalinating seawater, these typically require expensive infrastructure and lots of energy, putting them beyond

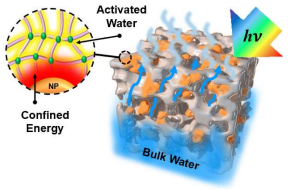
Solar vapor generation could be achieved under natural sunlight with large scale HNGs.

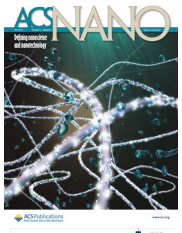
A seawater purification system has been demonstrated with potential daily yield of ~23 L/m^2.

Highly Tunable Material Platform for Solar Water Purification

- Integrating nanoscale solar absorber
- Managing heat loss

ACS Nano, 7913 (2019).

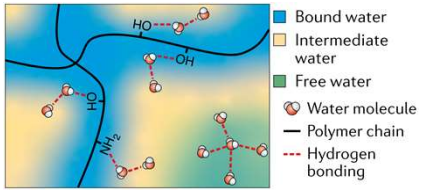




Energy utilization

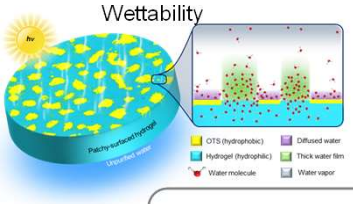
- Tuning hydrability of polymer
- Architecting polymer networks

Science Advances, aaw5484 (2019).



Polymer-water interaction

Nature Reviews Materials, 388 (2020).

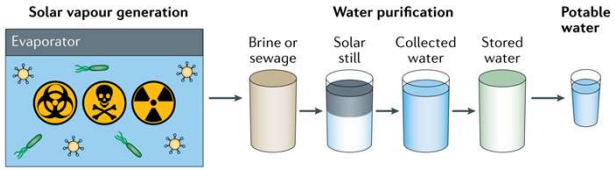


Interfacial study

Energy Environ Sci., 2087 (2020).

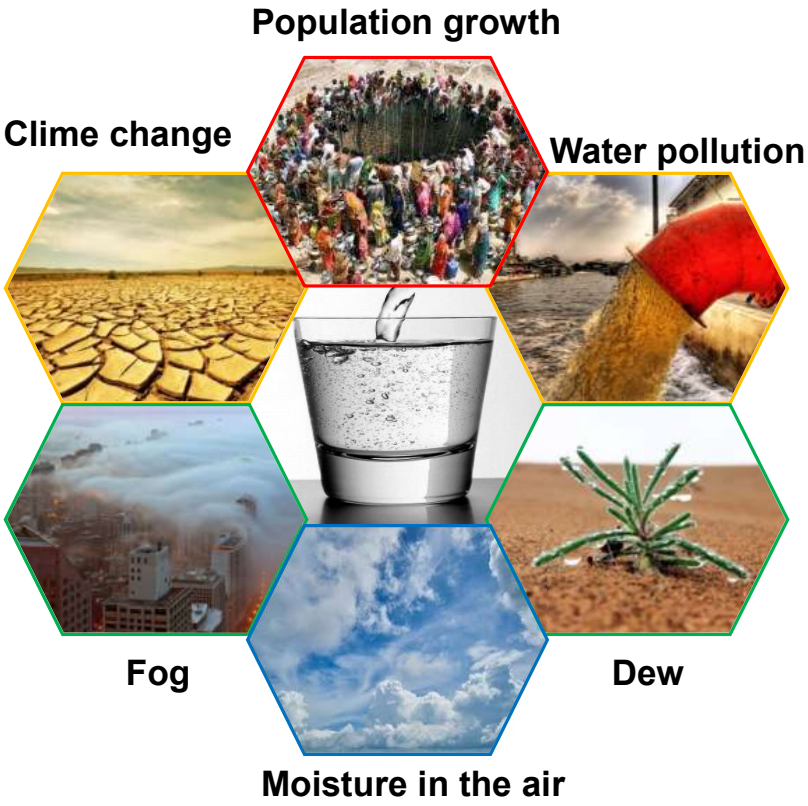
- Tuning surface topography
- Tuning surface wettability

Large-scale, portable devices



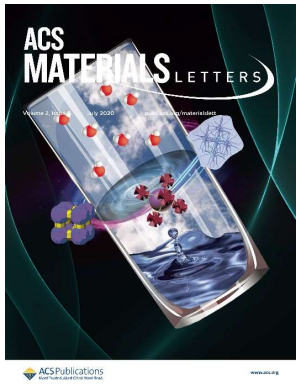
- Low-cost material/device
- Efficient water collection
- Quality monitoring

Atmospheric Water Harvesting (AWH)



- Land desertification and water pollution are worsening the situation
- Fog and dew can be directly collected as freshwater upon periodic temperature change
- Large amount of water is hiding in air for climatically and hydrologically independent freshwater production

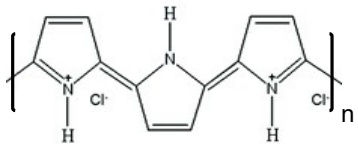
Atmospheric Water Harvesting



Zhou, Zhao, Yu, ***ACS Mater. Lett.*** 671 (2020).

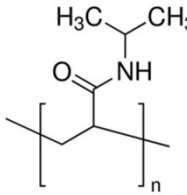
Super Moisture-Absorbent Gel (SMAG) for AWH

Hygroscopic polymer

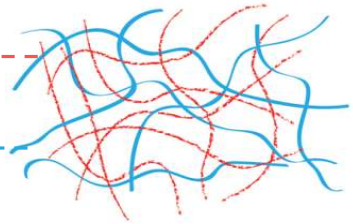


polypyrrole chloride
(PPy-Cl, 1st network)

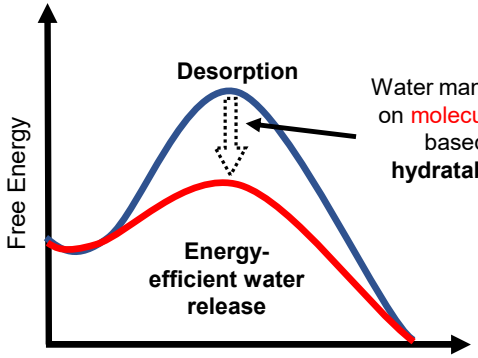
Hydrophilicity-switchable polymer



Poly(N-isopropylacrylamide)
(PNIPAM, 2nd network)

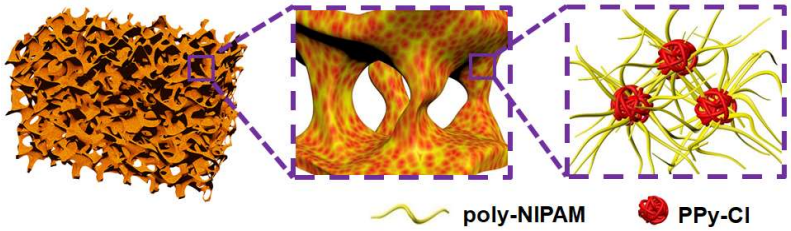


IPN

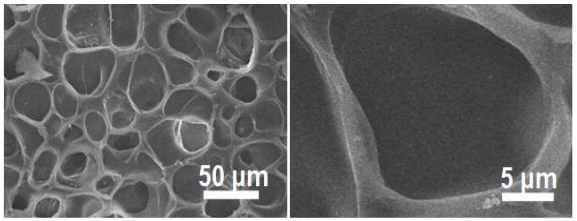


Water management on molecular level based on **hydratable** IPN

A novel material platform for AWH

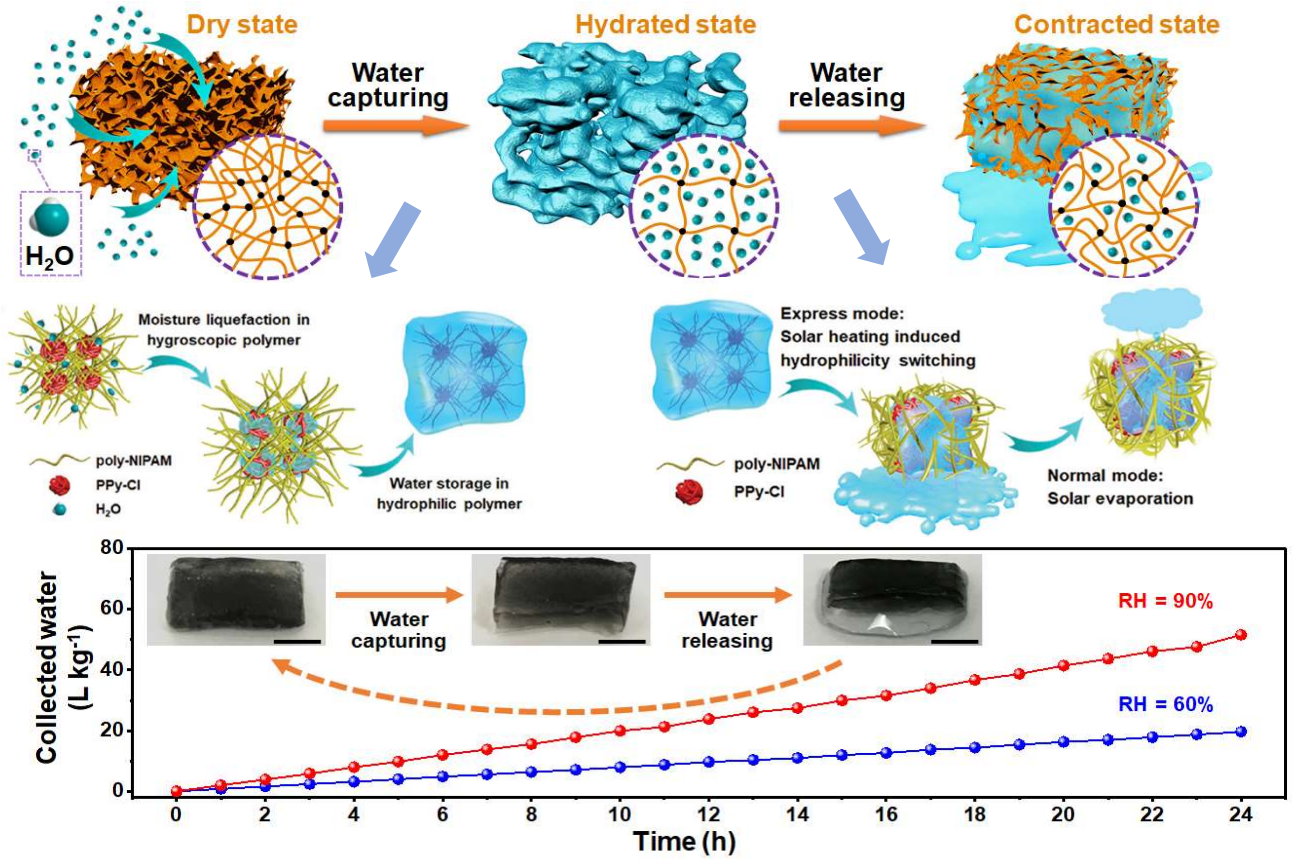


Porous structure



Zhao, Zhou, Yu, ***Adv. Mater.*** 1806446 (2019); ***Acc. Chem. Res.*** 3244 (2019).

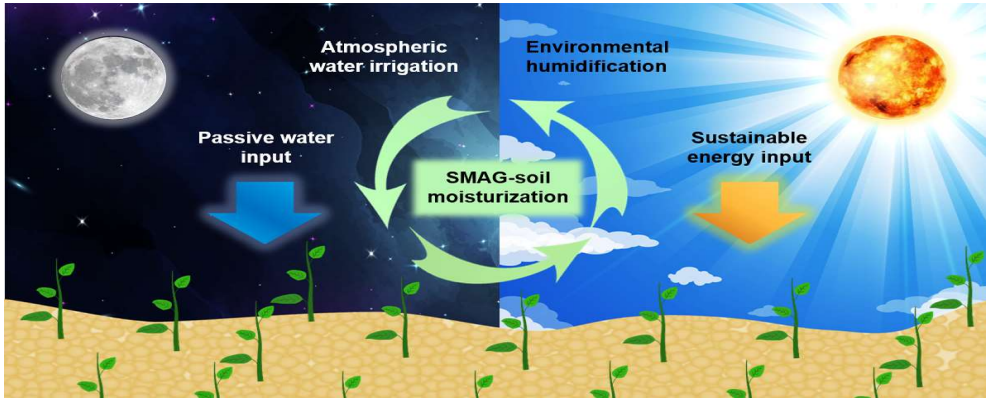
Highly Efficient Atmospheric Water Harvesting

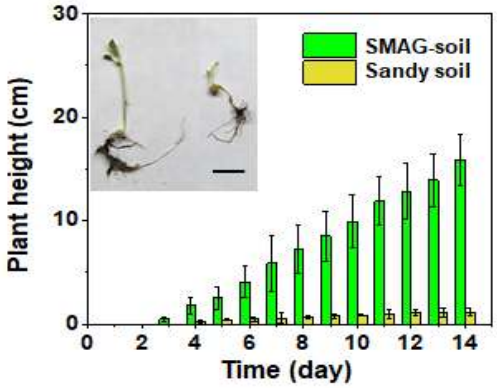


Solar-powered AWH with optimized water yield of 20~40 L kg^{-1} per day

Zhao, Zhou, Yu, ***Adv. Mater.*** 1806446 (2019);

Self-Watering Soil for Sustainable Agriculture





WORLD ECONOMIC FORUM

This new soil can water plants all by itself

The innovation could help increase farming potential in dry, deserted areas.

Image: REUTERS/Amit Dave

- SMAG-enabled atmospheric water irrigation for plant growth under very dry and hot conditions
- Irrigation-free planting with high germination and survival rate over 95%

Zhou, Yu, ***ACS Mater. Lett.*** 1419 (2020).

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Yu Research Group @ UT Austin

Over the past years:

25 Undergrad Researchers
23 Graduate Researchers
13 Postdoc Researchers
9 Visiting Scholars

Current group:

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