COFS

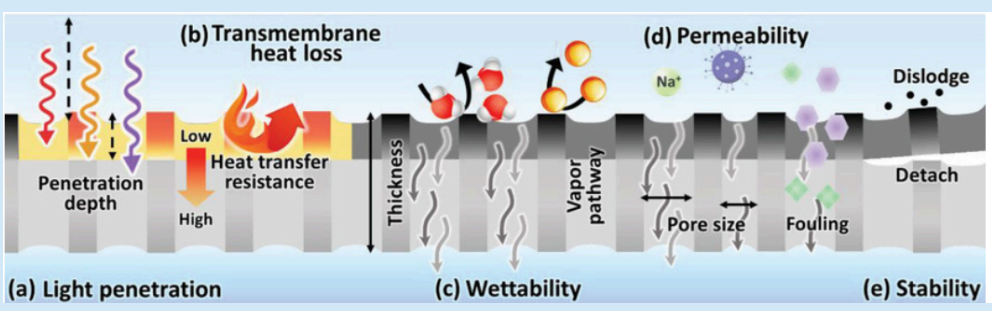
FOR PHOTO-THERMAL MEMBRANE DISTILLATION

Infographic by: Alex Gnaedinger (Civil Engineering) / **Produced on:** September 9th, 2024 / **Supervised by:** Dr. Heather Buckley

01 The Goal: Produce Clean Water from Sunlight

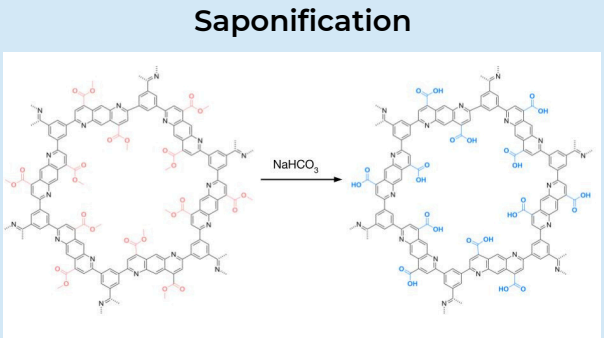
Photothermal membrane distillation uses sunlight to produce clean water through the following steps:

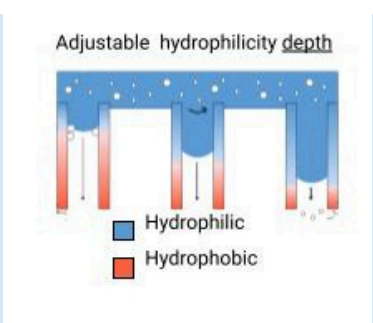
- Feed-water adsorbs onto a hydrophilic membrane layer.
- The membrane converts solar radiation to heat, vaporizing the adsorbed water.
- Vapor penetrates a hydrophobic membrane layer and condenses on the other side.



Small Methods 2021, 5 (5), 2001200.

Adjustable Hydrophilicity of COF via Saponification





Aasen, K. *Hydrophilicity Gradient in COF.* PowerPoint Presentation, Unpublished, 2024.

02 Why use COFs?

Covalent Organic Frameworks (COFs) are ideal for membrane materials due to:

- **Ordered Structure:** Self-correction through reversible reactions during formation.
- **Tunable Properties:** Adjustable pore size, hydrophilicity, and photothermal conversion.
- **Green Chemistry Compatible:** Solvent-free synthesis and green building blocks.

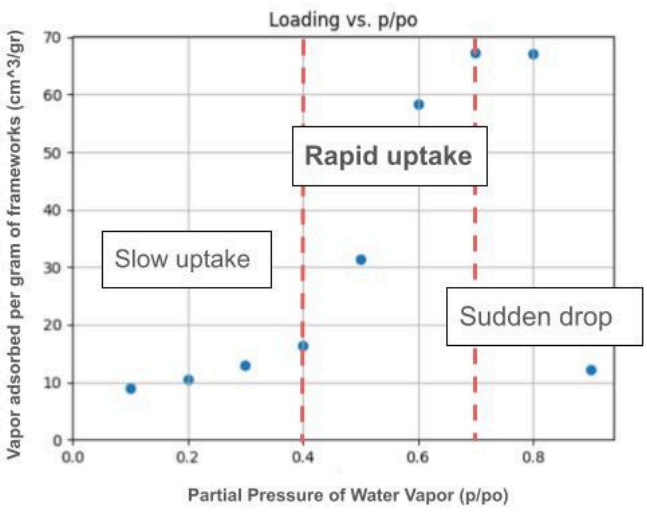
03 Screening Structures

We used molecular simulation to identify promising COF structures. Simulations predict important characteristics efficiently, saving time and energy compared to in-lab synthesis.

How?
RASPA adsorption simulation software implements algorithms to predict structural properties of COFs and model interactions with adsorbate molecules.

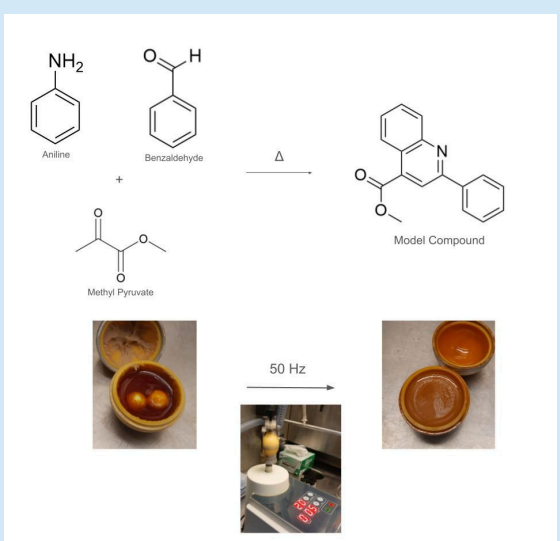
Isotherm: Shows gas adsorption to the framework at various pressures, indicating material hydrophilicity.

Modelled Isotherm of COF TpPa-1



Hydrophilic: Rapid uptake at low to moderate relative humidity

Mechanochemical Synthesis of a Quinoline Based Model Compound



04 Synthesis of Model Compounds

Mechano-chemical synthesis uses the kinetic energy from grinding balls to drive reactions, eliminating the need for heat and solvents.

We chose it over traditional methods because it:

- Uses no toxic solvents
- Requires less time and energy

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