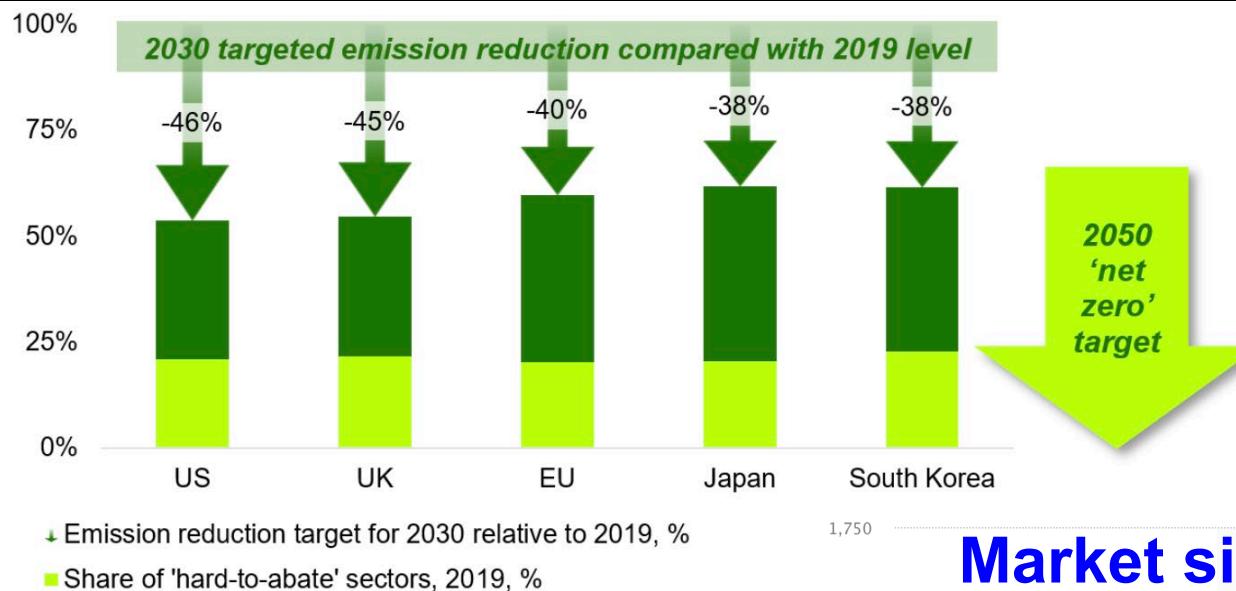


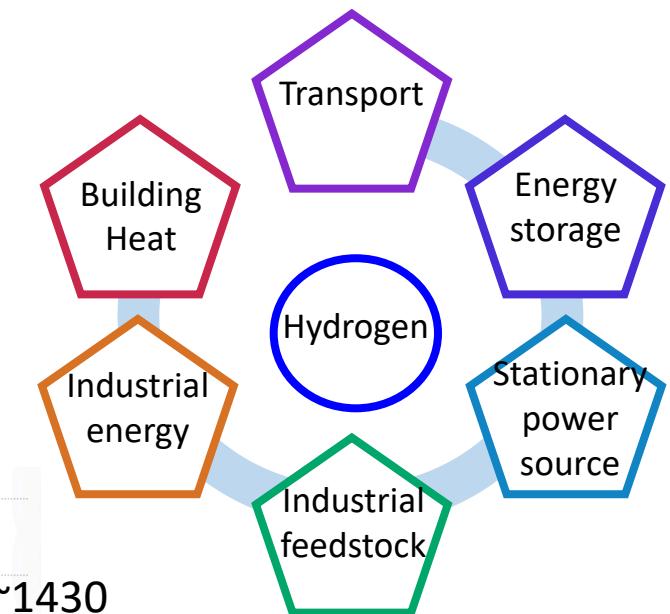
Neutrons: a journey through green energy

Fabrizia Foglia

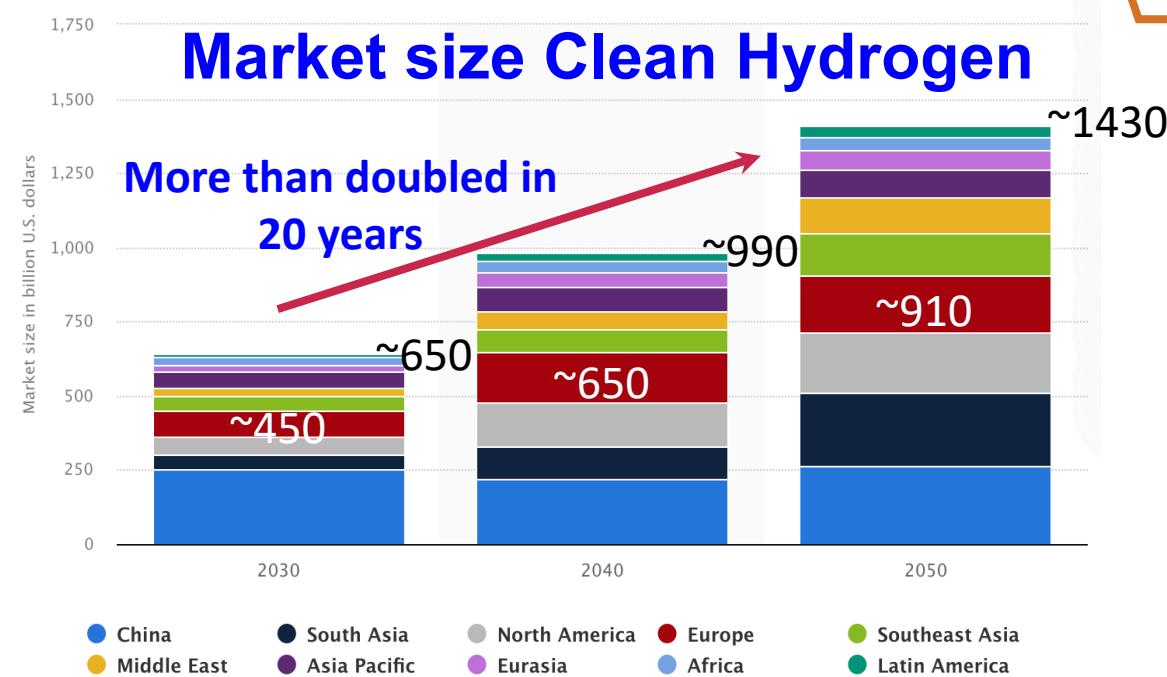
f.foglia@ucl.ac.uk



2050
'net
zero'
target



Market size Clean Hydrogen



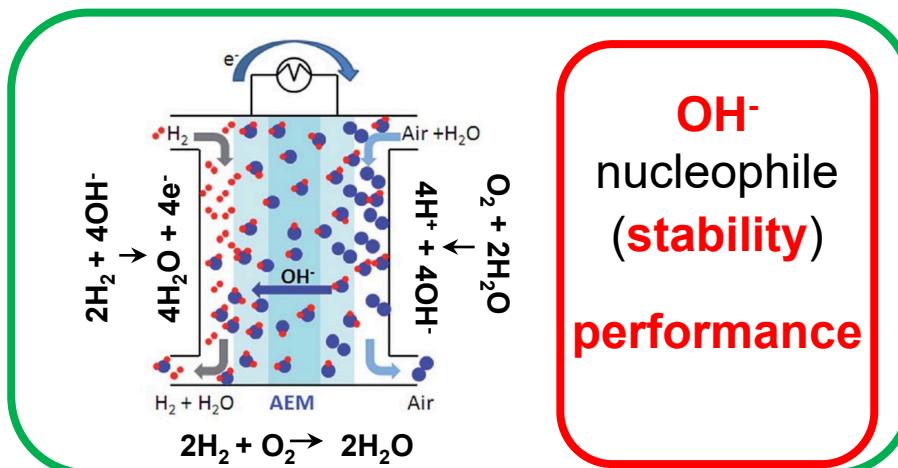
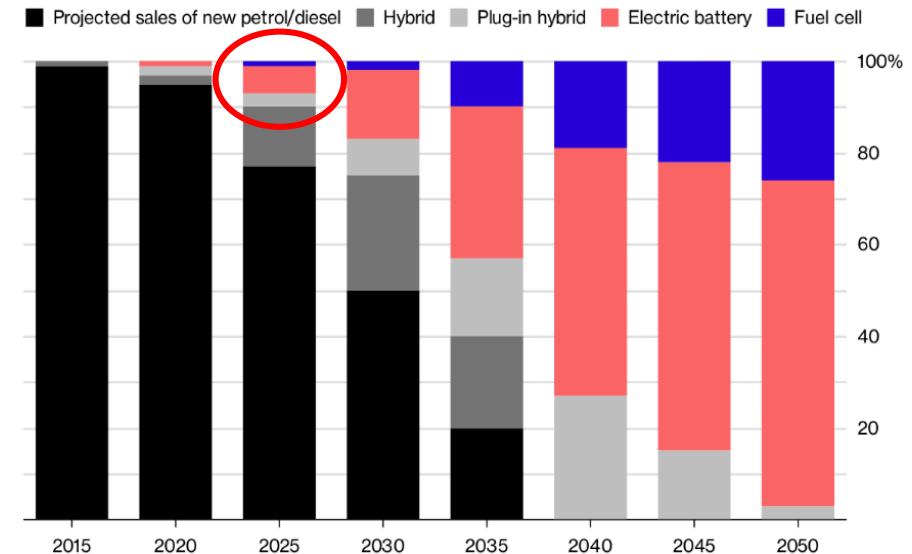
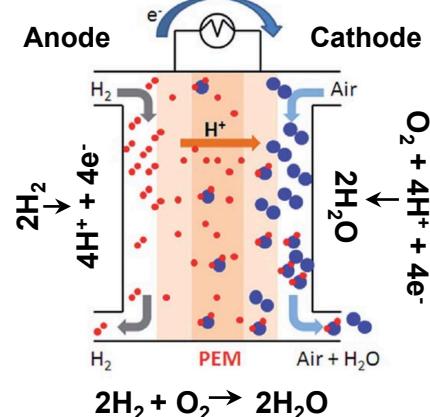
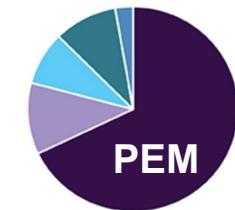
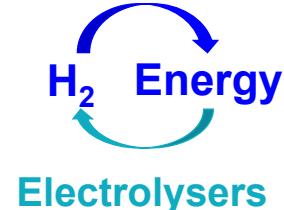
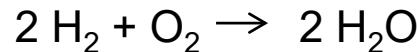
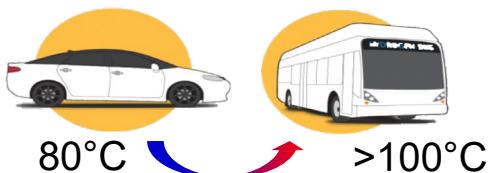
FUEL CELLS

Environmentally friendly

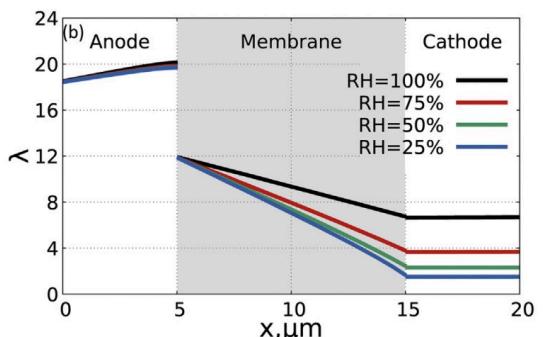
- i) water is the byproduct of the electrochemical reaction in a fuel cell (ideal candidate in the quest for fighting climate change);

Cons

- i) Pt-based catalysts (**expensive**).
- ii) the cell performance is affected by the **water content**;
- iii) at **low-T** (60-80°C) it is necessary to eliminate CO to avoid catalyst poisoning.

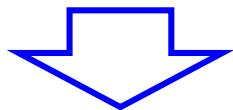


OH⁻ nucleophile (stability) performance

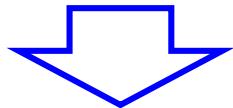


DR Dekel, et al, J Power Sources 375, 191 (2018)

Design

HIGH-PERFORMING MEMBRANES

explicate the
structure-to-function interplay



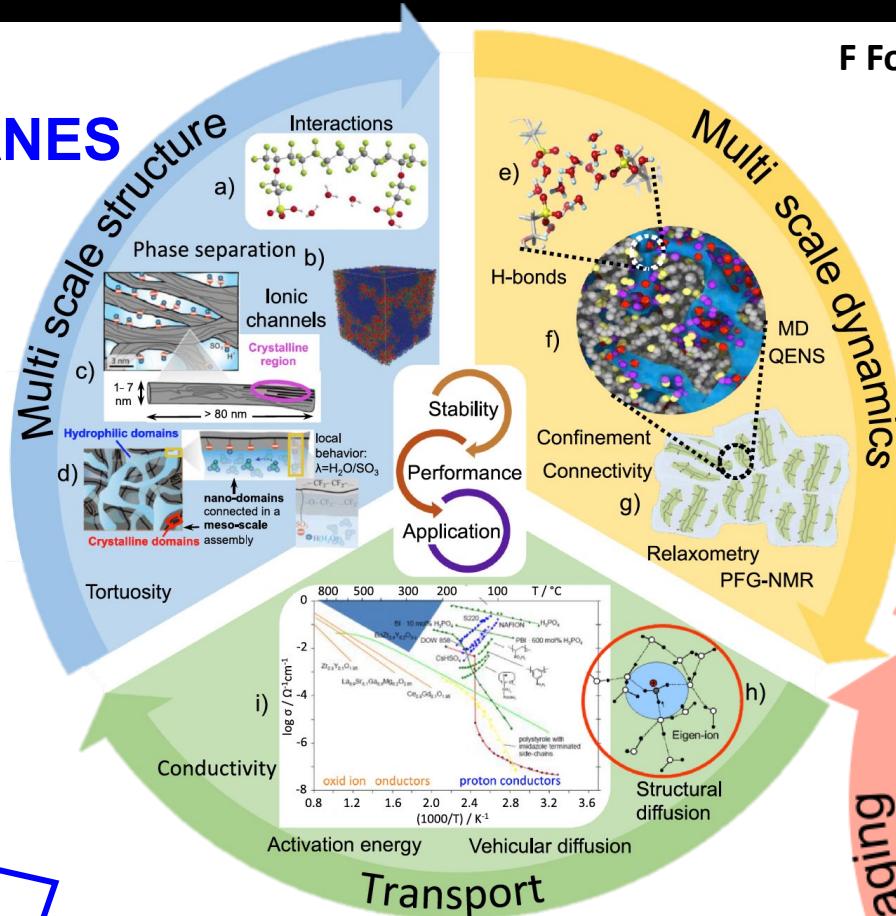
disentangle processes
(within polymer & solute)



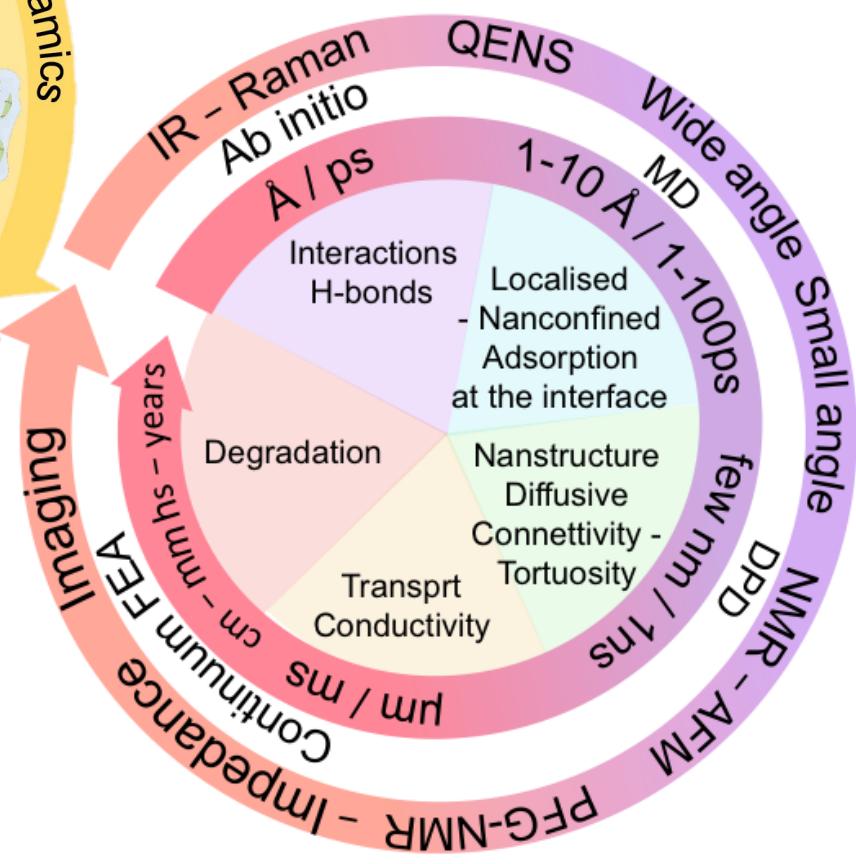
holistic approach



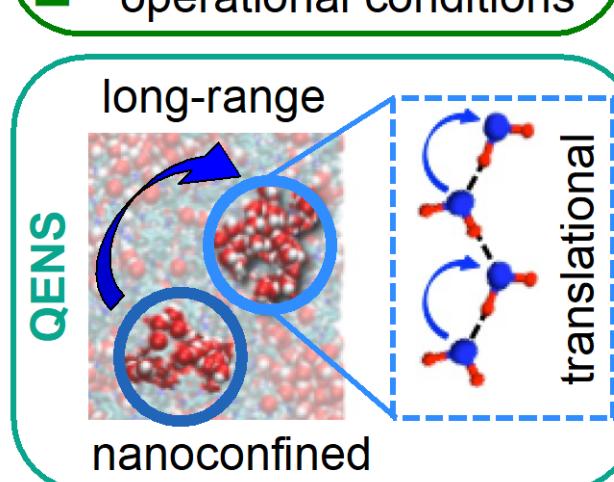
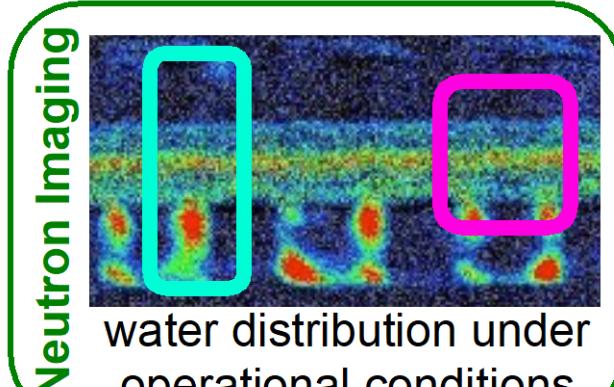
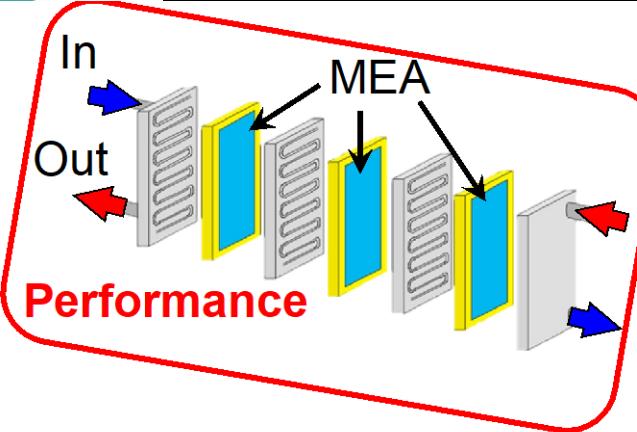
Industrial requirement & demands



F Foglia*, et al, *J Non-Crystalline Solids: X*
13 100073 (2022)



HIGH-PER



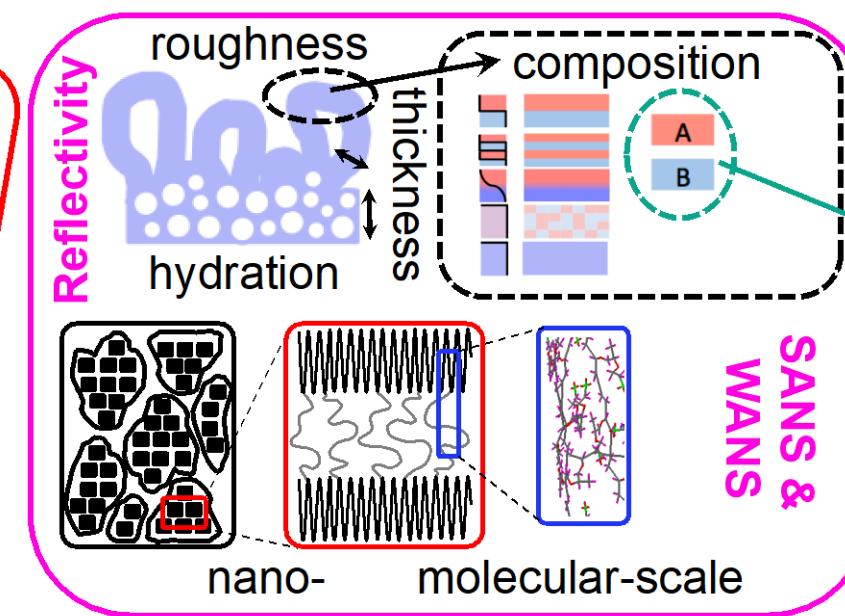
structure-

disent

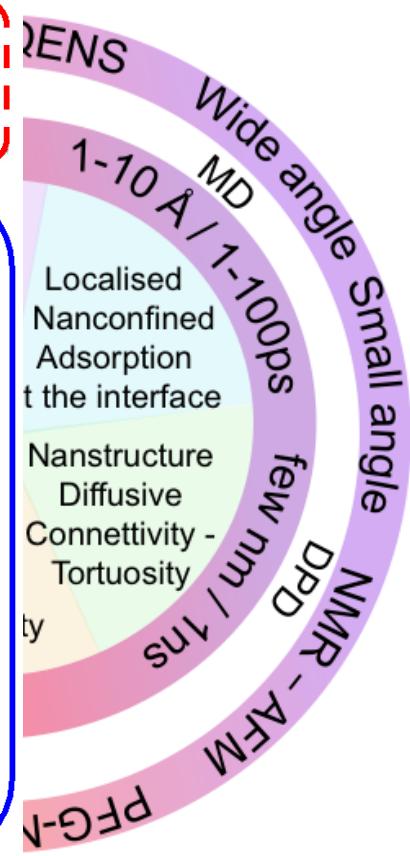
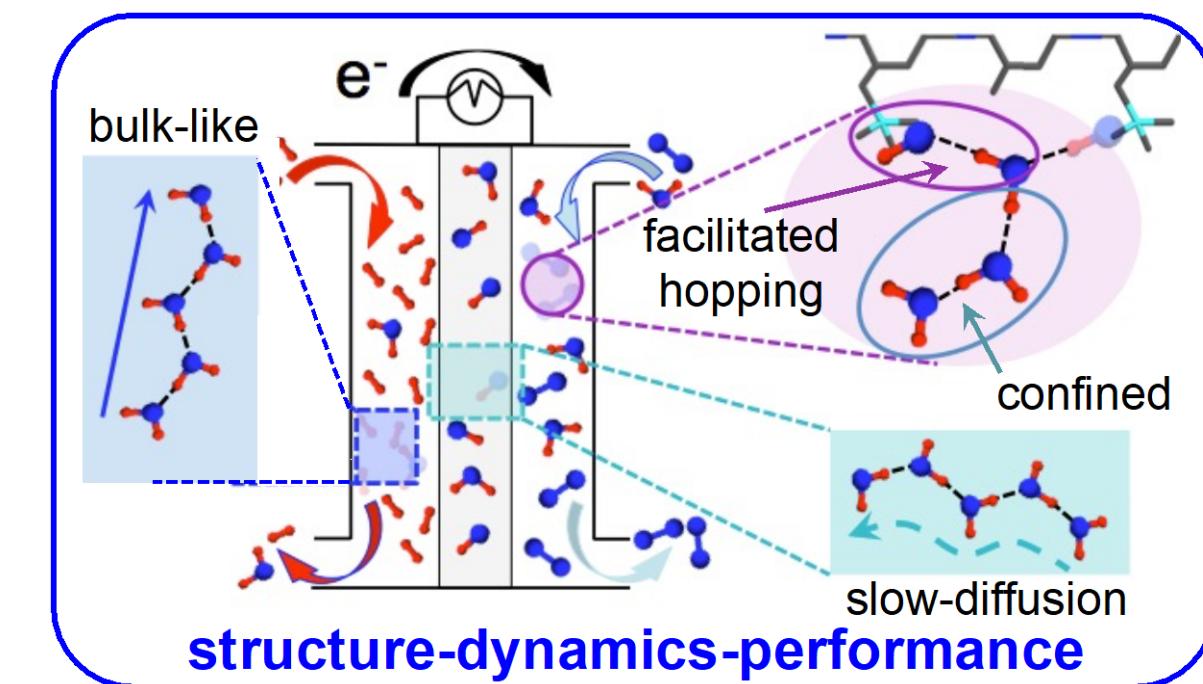
(within)

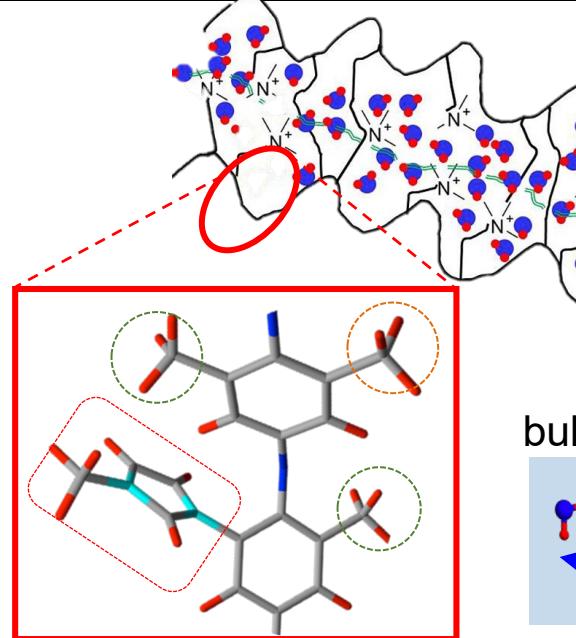
holis

Industrial



relaxation &
geometry of
the movement





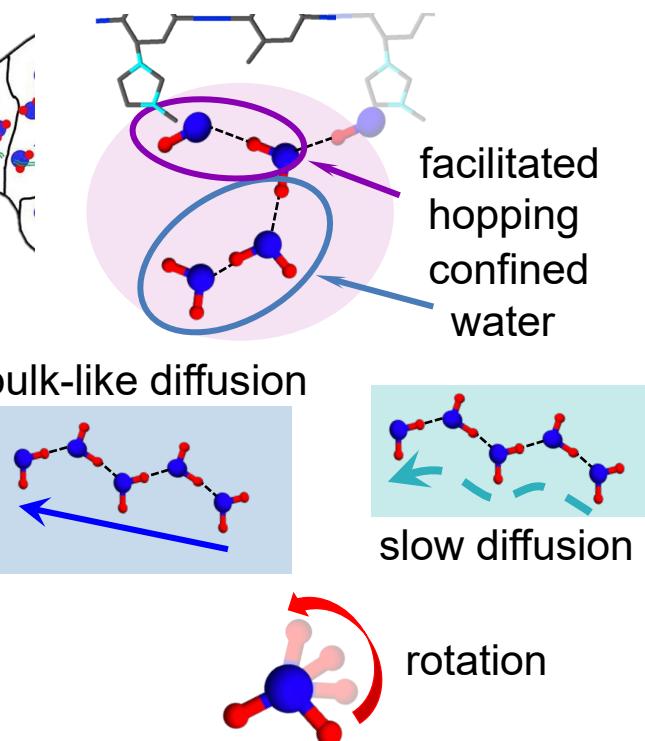
a few (coupled) dynamics:

- Polymer**
- $-\text{CH}_3$ rotation
 - backbone relaxation

- Ion**
- facilitated hopping

- rotation

- Water**
- c-o-m diffusion
 - confinement



disentangling dynamics

time

$\sim 0.5 \leq \tau \leq 20 \text{ ps}$
 $E_{\text{res}} = 70 \mu\text{eV}$
IN6

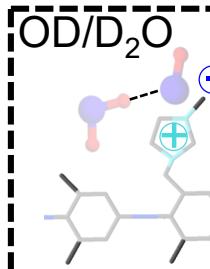
$\sim 5 \leq \tau \leq 100 \text{ ps}$
 $E_{\text{res}} = 17.5 \mu\text{eV}$
IRIS

$\sim 0.07 \leq \tau \leq 3 \text{ ns}$
 $E_{\text{res}} = 0.75 \mu\text{eV}$
IN16B

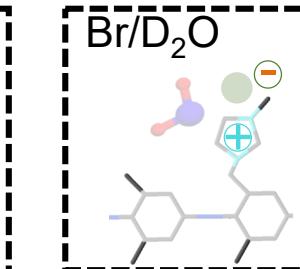
$E_{\text{res}} = 1.0 \mu\text{eV}$
HFBS

composition (/dynamics)

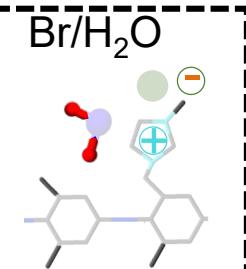
OD/D₂O



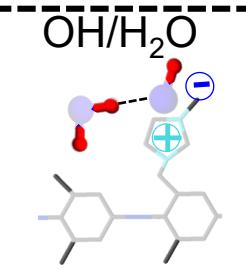
Br/D₂O



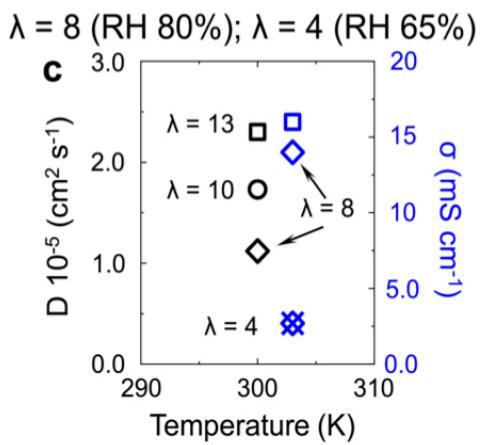
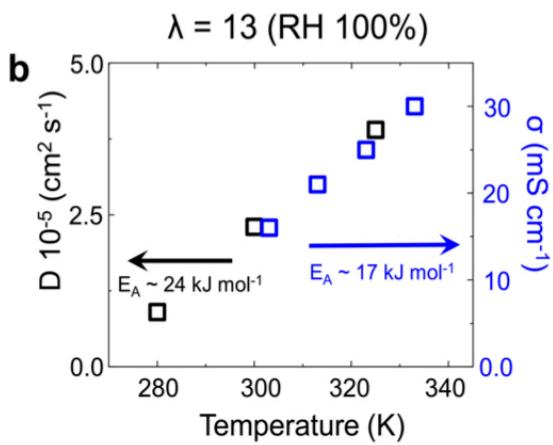
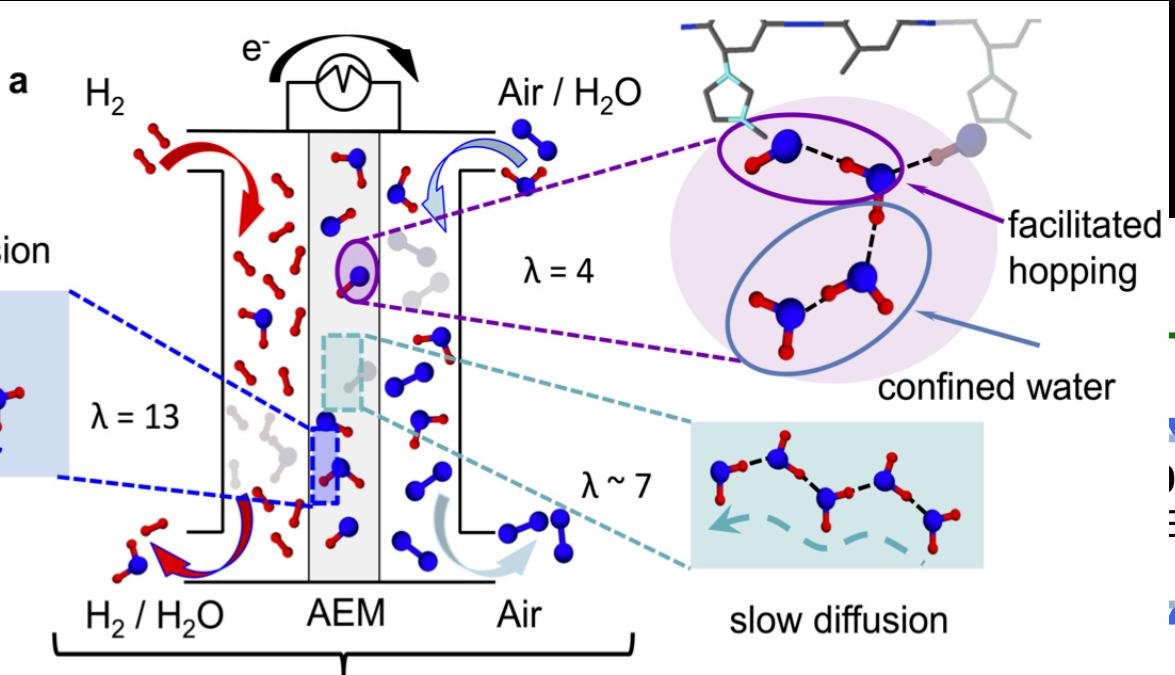
Br/H₂O



OH/H₂O



water content (λ)



F. Foglia* et al. *Nature Materials* **21** 555 (2022)

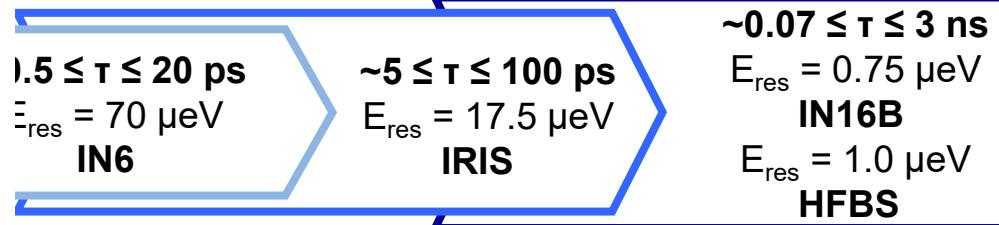
understanding
from atom to
application



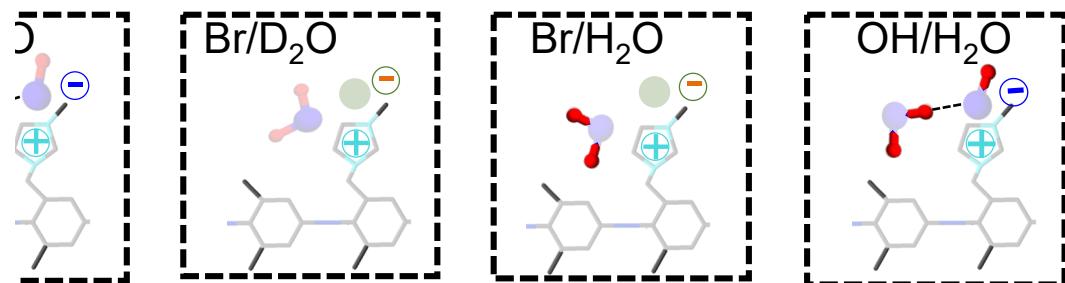
correlate dynamics parameters to performance



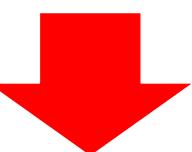
disentangling dynamics



position (/dynamics)



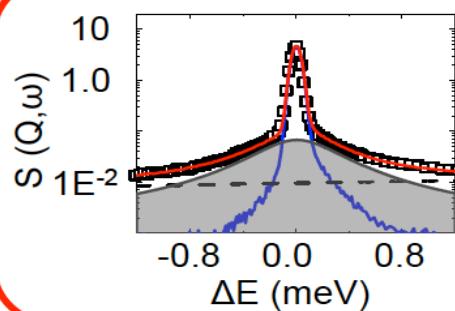
content (λ)



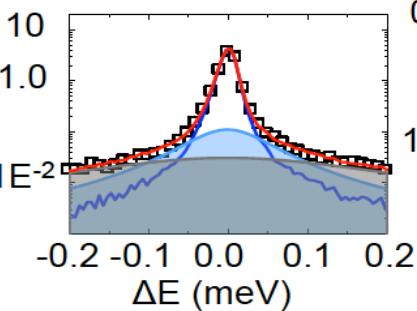


Polymer

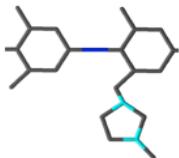
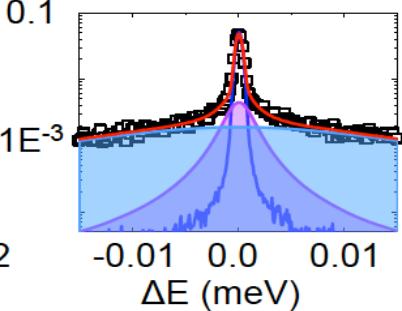
$\lambda = 4; 300 \text{ K}$



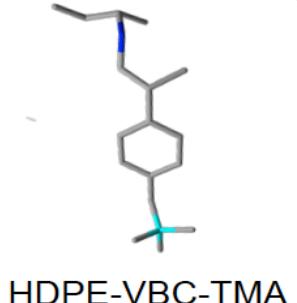
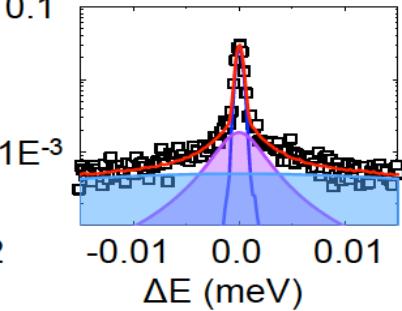
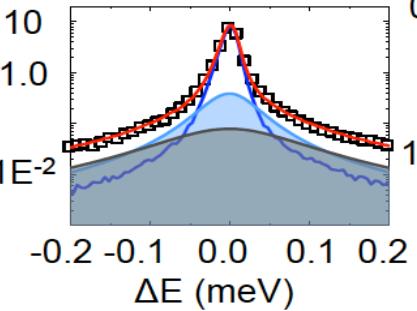
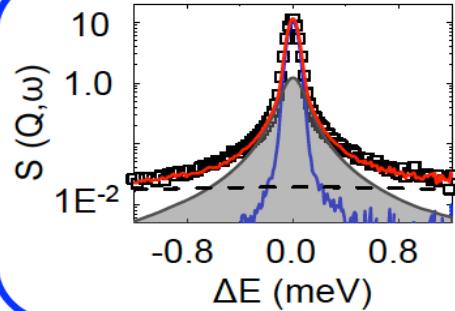
Polymer & Water



Polymer + Water & Facilitated OH⁻ hopping



FAD

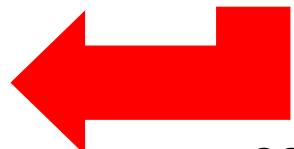


HDPE-VBC-TMA

BROAD
IN6 - $E_{\text{res}} = 70 \mu\text{eV}$
($\sim 0.5 \leq \tau \leq 20 \text{ ps}$)

INTERMEDIATE
RESOLUTION
IN16B - $E_{\text{res}} = 0.75 \mu\text{eV}$
($\sim 0.07 \leq \tau \leq 3 \text{ ns}$)

understanding
from atom to
application



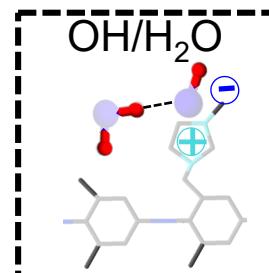
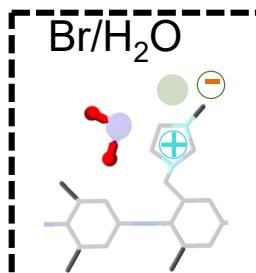
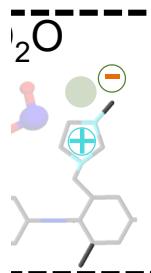
correlate dynamics parameters to performance

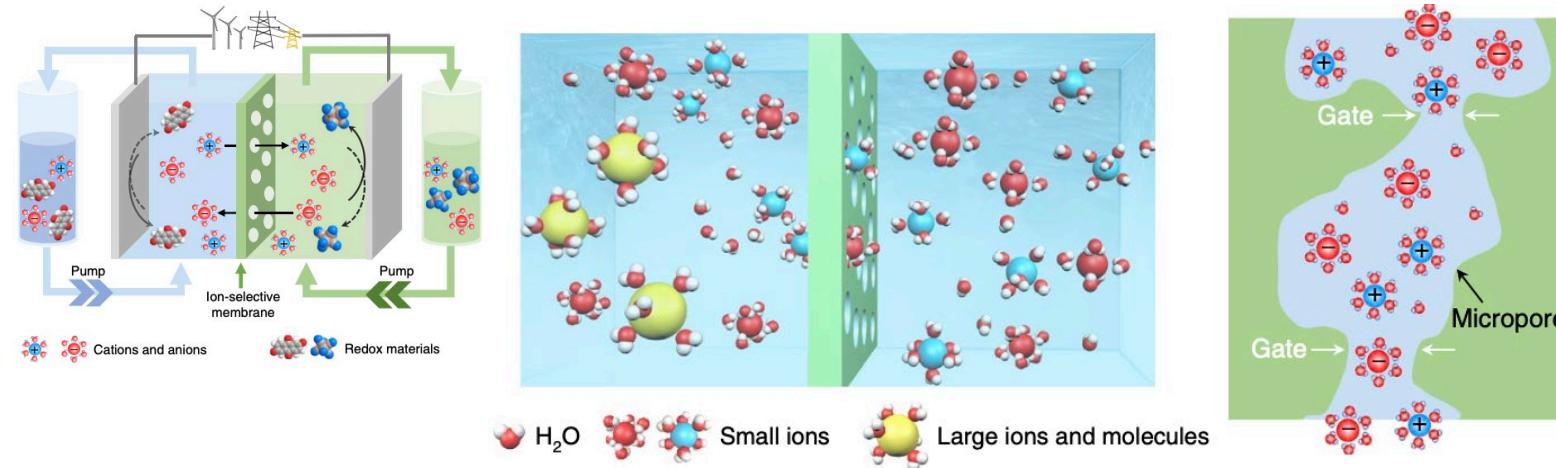
entangling dynamics

$\sim 5 \leq \tau \leq 100 \text{ ps}$
 $E_{\text{res}} = 17.5 \mu\text{eV}$
IRIS

$\sim 0.07 \leq \tau \leq 3 \text{ ns}$
 $E_{\text{res}} = 0.75 \mu\text{eV}$
IN16B
 $E_{\text{res}} = 1.0 \mu\text{eV}$
HFBS

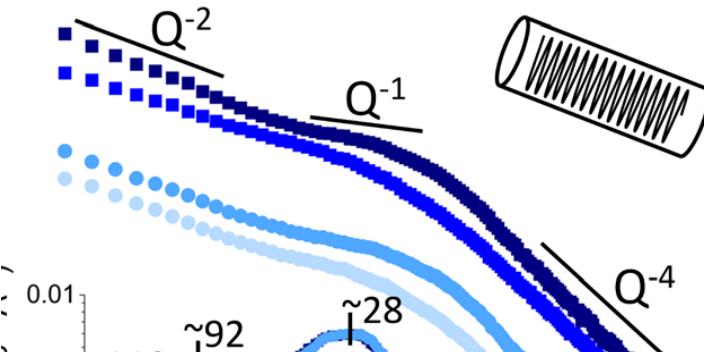
dynamics)



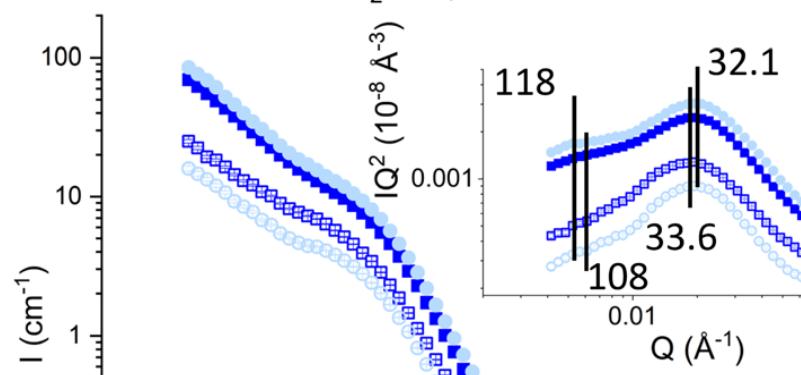


Radiation-grafted anion-exchange membranes for CO₂ electroreduction cells

- MPIP(LEX) dry
- MPIP(1.1) dry
- MPIP(LEX) H₂O-hydrated
- MPIP(1.1) H₂O-hydrated

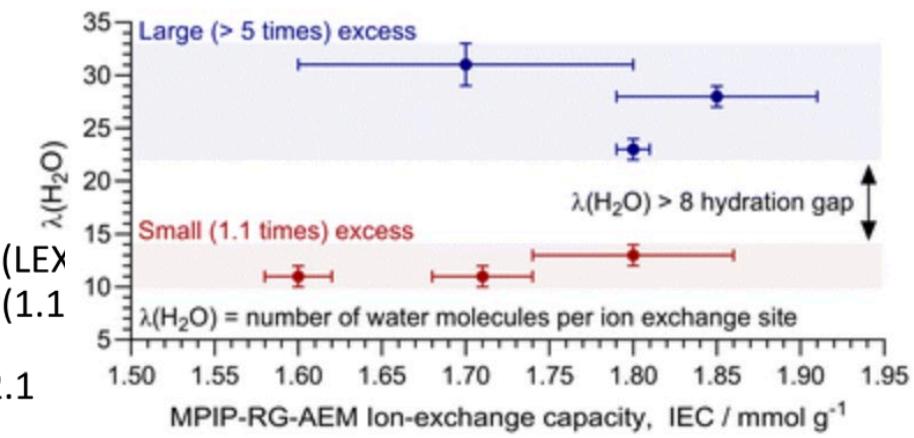


- MPIP(LEX) H₂O-hydrated
- MPIP(1.1) H₂O-hydrated
- MPIP(LEX) dry
- MPIP(1.1) dry



R. Tan et al. *Nature Materials* **19** 195 (2020)
A. Wang et al. *Nature* submitted

Redox-flow batteries



T. Willson et al. *J. Mater. Chem. A*
11 20724 (2023)

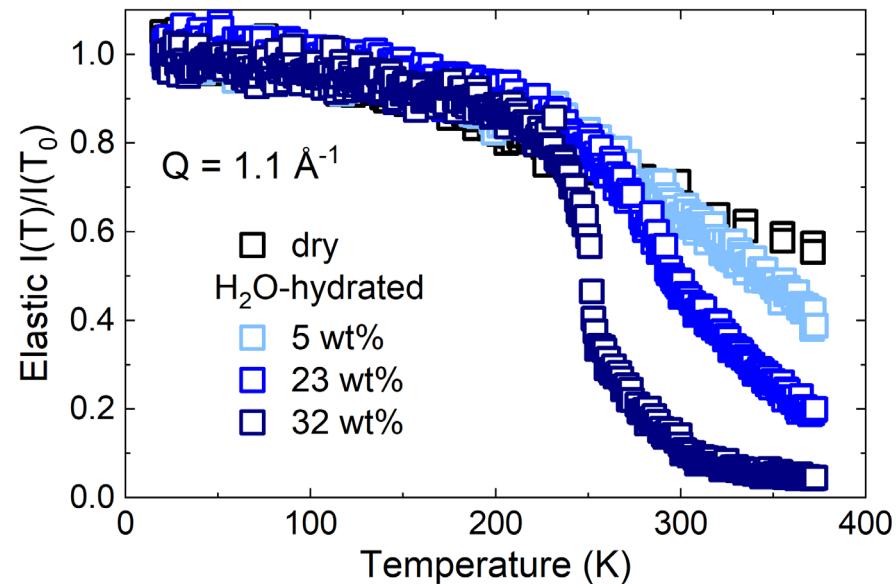
**Nafion****Low-T FC**
 $T \leq 80^\circ\text{C}$

Bypass water management issues, low fuel flexibility, and a relatively fast degradation.

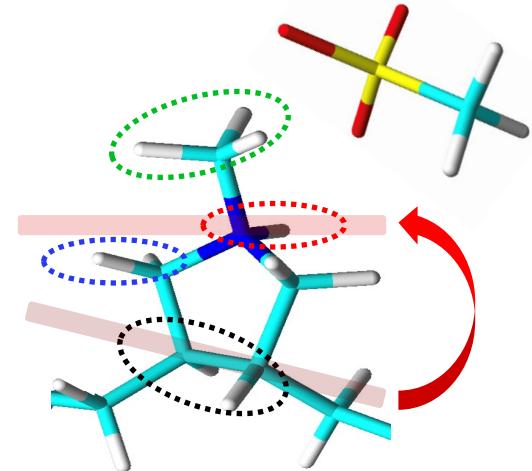
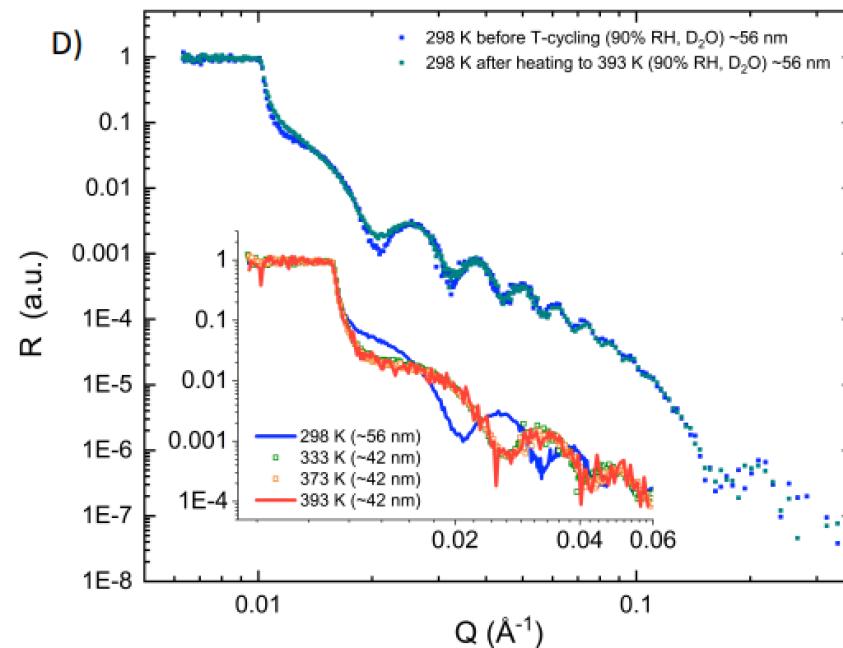
Intermediate-T FC $100 \leq T \leq 120^\circ\text{C}$ **High-T FC**
 $140 \leq T \leq 200^\circ\text{C}$

Develop a suitable PEM with comparable performance and lifetime to Nafion.

- improve:
- mechanical strength
 - water retention
 - enhance proton conductivity



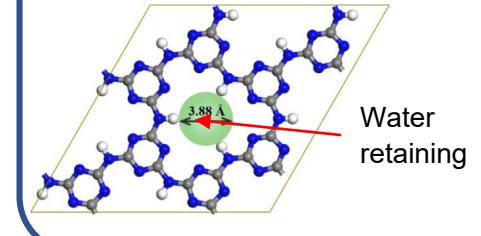
Polymat – Toyota: Develop new chemistries



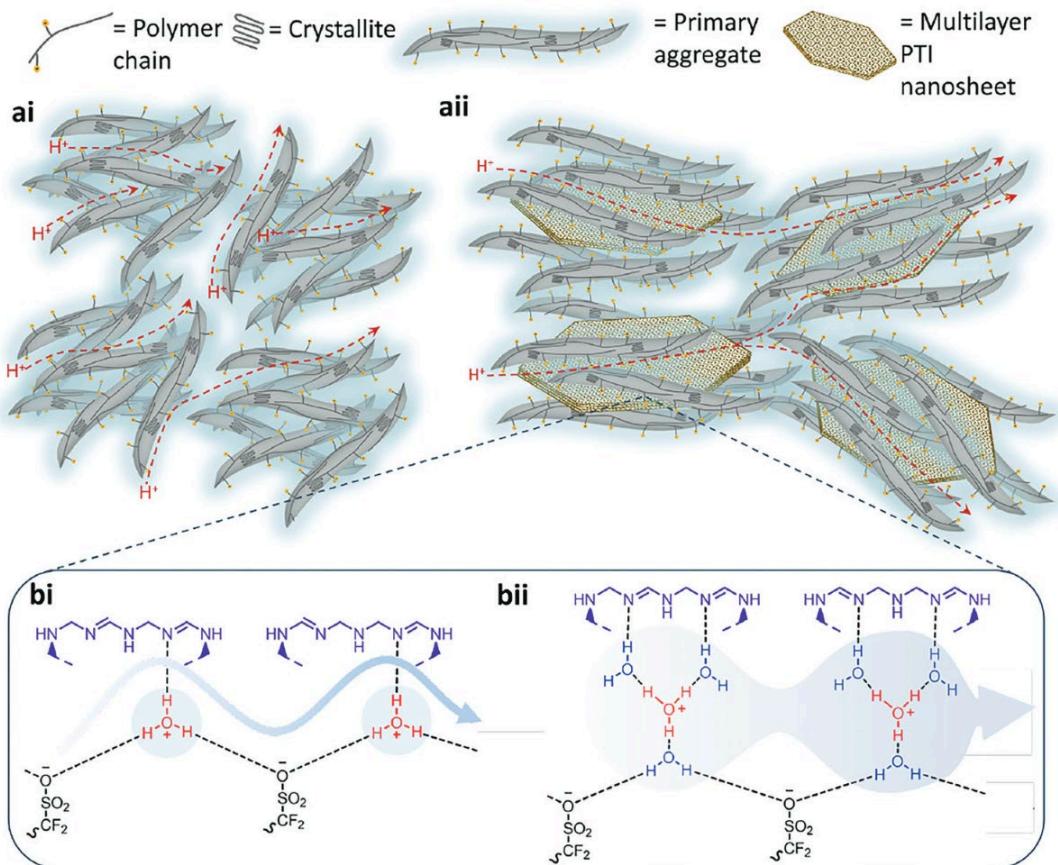
Polymat (& Toyota Motor Europe) has developed new chemistry for operation at intermediate-T conditions. We are testing the properties of this material **to improve performance**.

CEA – EIL: Nanocomposite
membranes (Nafion + fillers)

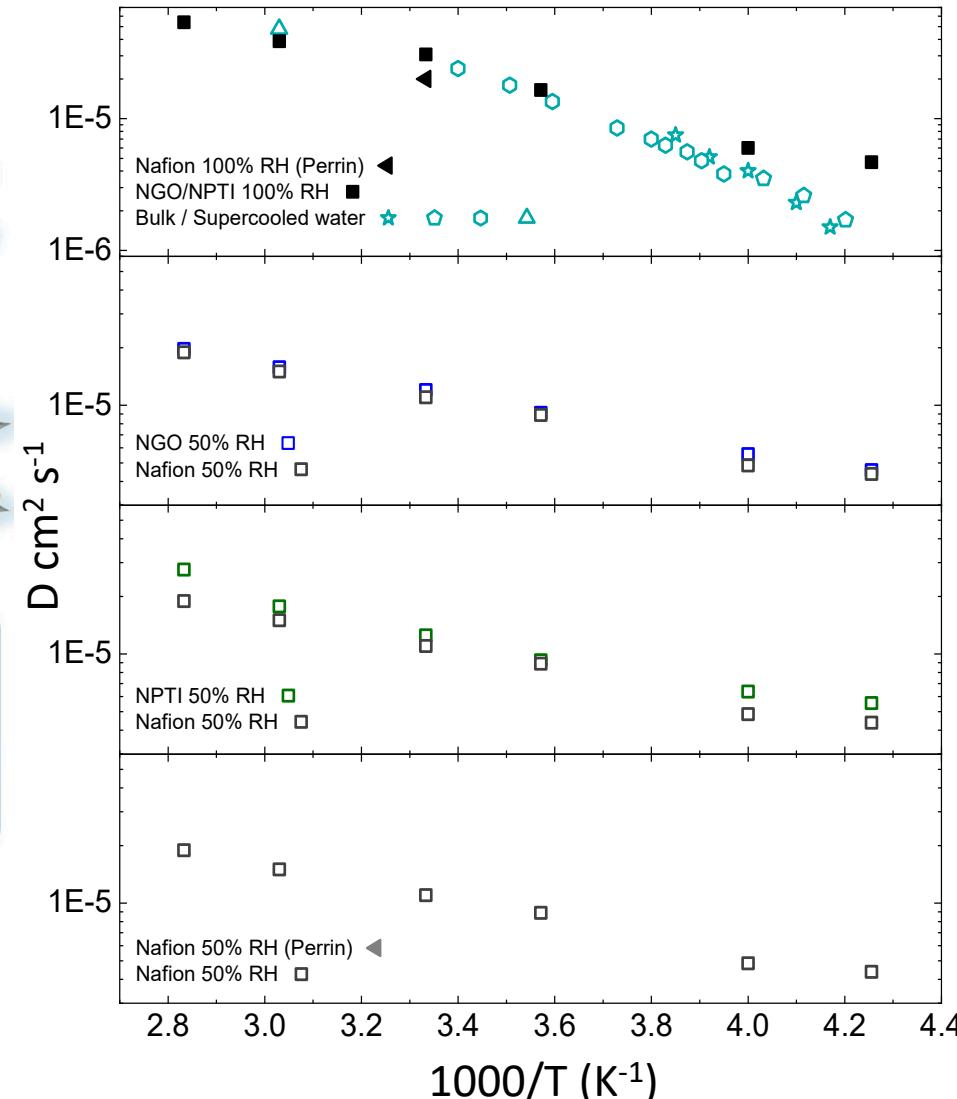
Polytriazine imide (PTI)

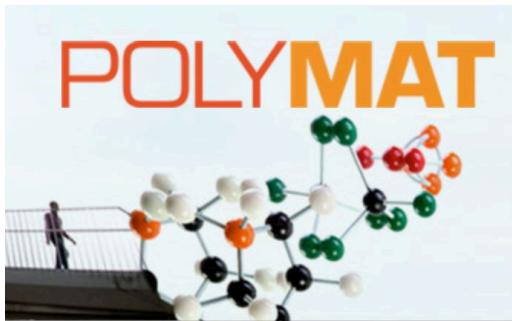


K Smith et al, Advanced
Functional Materials
2304061 (2023)



The addition of C-material within Nafion enhancing the diffusivity improve performance at low-RH.





Science & Technology Facilities Council
ISIS

Imperial College
London



Acknowledgment



electrochemical
innovation
lab

