

Knowledge transfer
from membrane science to
battery applications

Enabling Nano-architected Thin Films to Enhance Lithium- sulfur Battery Performance

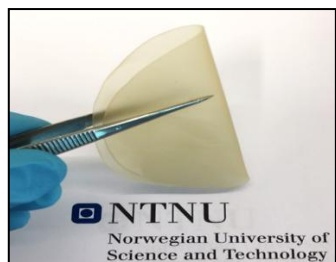
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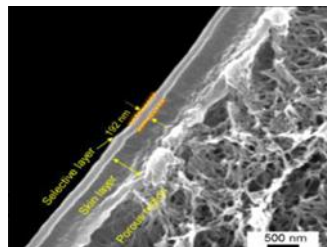


Background

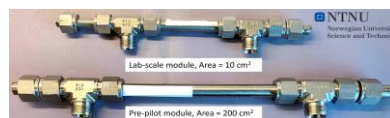
Membrane development path



Membrane materials optimization



Thin composite membranes (flat sheet)



Module fabrication & industrial validation

Industry process



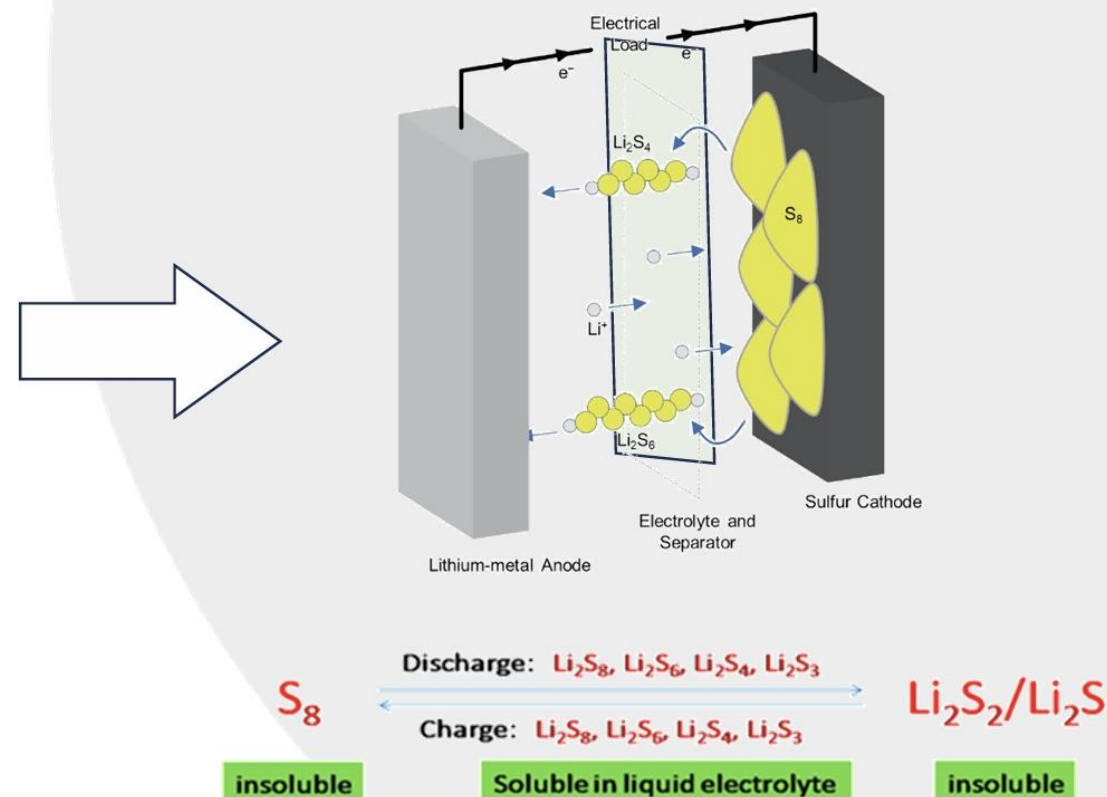
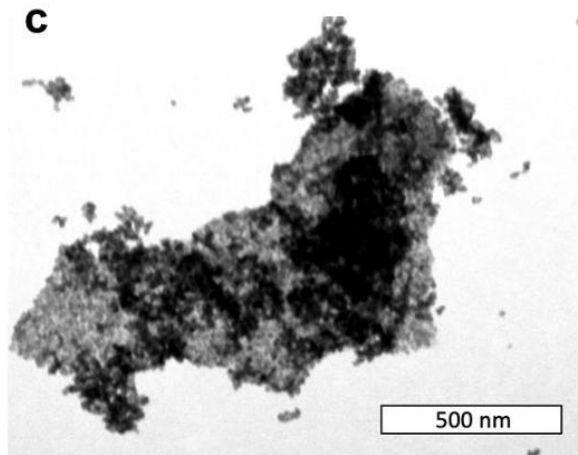
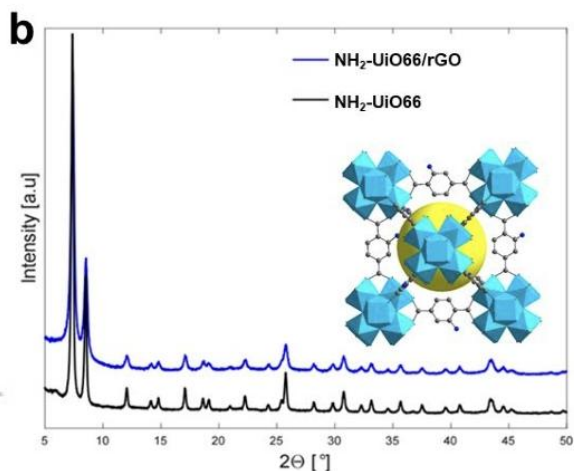
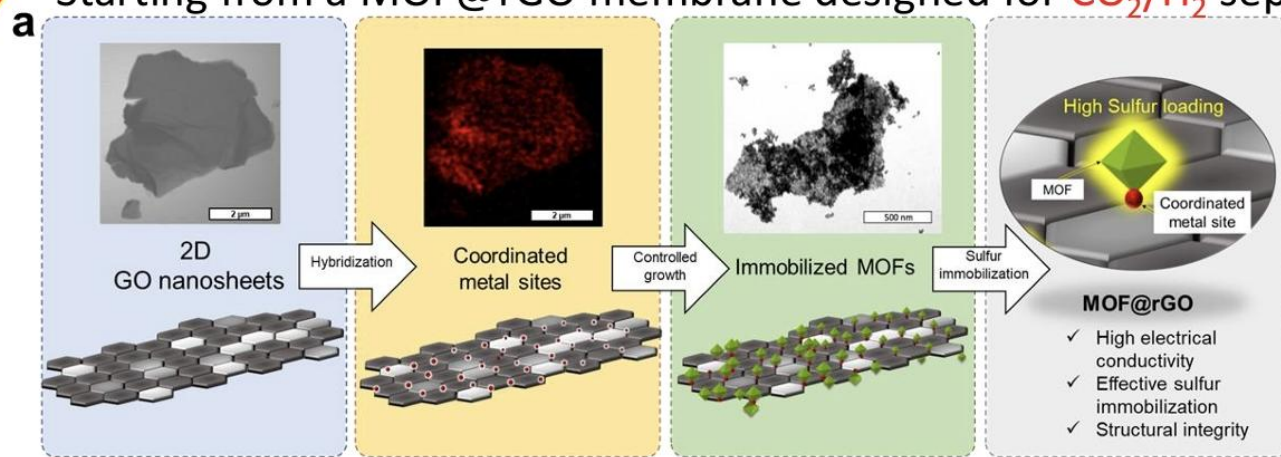
Pilot-scale test



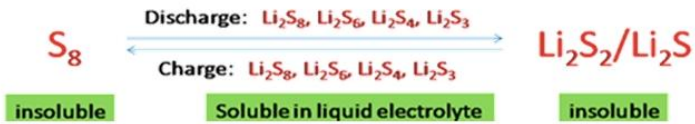
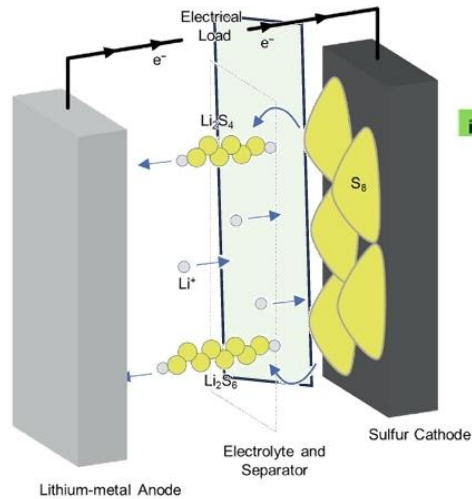
Thin composite membranes

Inspired by a special nanostructured membrane - our path towards Lithium-Sulfur batteries!

Starting from a MOF@rGO membrane designed for CO_2/H_2 separation



Li-S batteries: **Advantages** and challenges



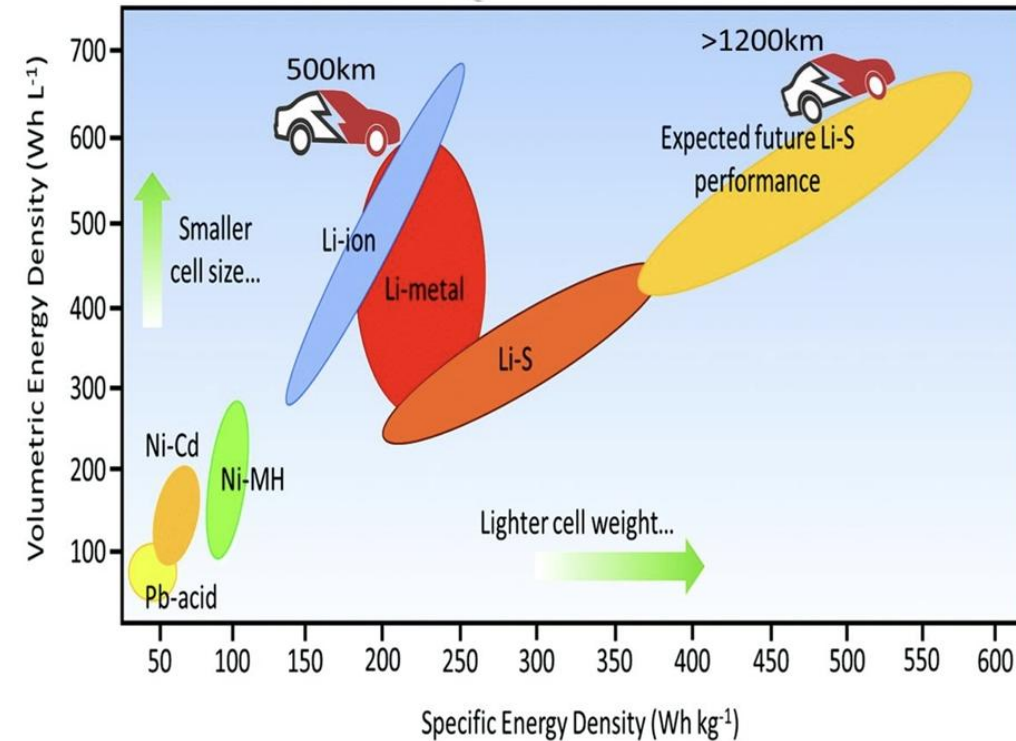
Conversion reactions: forming new materials during charge and discharge



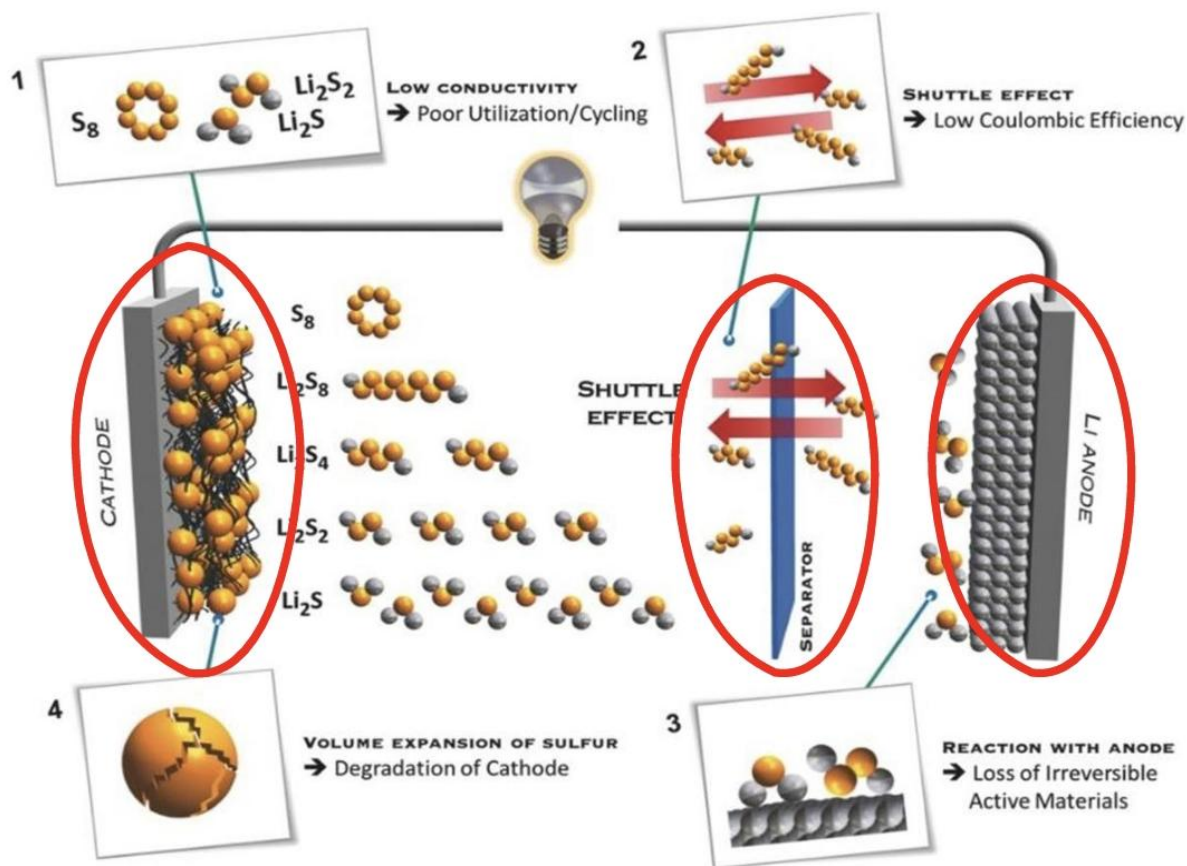
Advantages

- ✓ High theoretical specific capacity ($5 \times LiB$)
- ✓ High specific energy
- ✓ Lightweight
- ✓ High charge rate capacity
- ✓ Improved safety
- ✓ Reduced material cost
- ✓ Low battery failure risk

Li dendrite formation



Li-S batteries: Advantages and challenges



Advantages

- ✓ High theoretical specific capacity (5×LiB)
- ✓ High specific energy
- ✓ Lightweight
- ✓ High charge rate capacity
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- ✓ Reduced material cost
- ✓ Low battery failure risk

- ✗ Short cycle life
- ✗ Low efficiency
- ✗ Low stability

- ✗ Polysulfide shuttle effect
- ✗ Low conductivity in cathode
- ✗ Cathode expansion
- ✗ Deactivation of anode

Yang, L., et al., *Ionics*, 2020. 26, 5299.

Lagadec, M.F., et al., *Nature Energy*, 2019. 4(1): p. 16-25

Li_2S_n :	0.5-1.5nm
Li^+ :	0.076nm

Our membrane-inspired solutions to those issues

Technology conversion and convergence:

→ From membranes to separators and cathode materials for long life Li-S battery

- **Nanosturctured cathode materials**



→ **MOF@rGO**

MOGLiS: MOF@rGO-based cathodes for Li-S Batteries



Dr. Rameez Razaq



Dr. Saravanan Janakiraman

- **MOGLiS project**

- **Mutlifunctional nanomaterials**



→ **Bimetallic MOF-based separator**

3S Battery: Super Selective Separators for Battery Applications



Dr. Önder Tekinalp

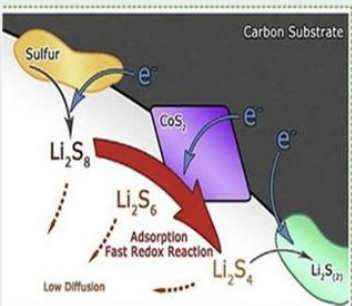


Ms Zainab Waris

- **3S Battery project**

Poster presentations →

MOGLiS: MOF@rGO-based S cathode concept



Amine group

- ✓ Affinity to polysulfides (Chemical confinement)

Porous structure

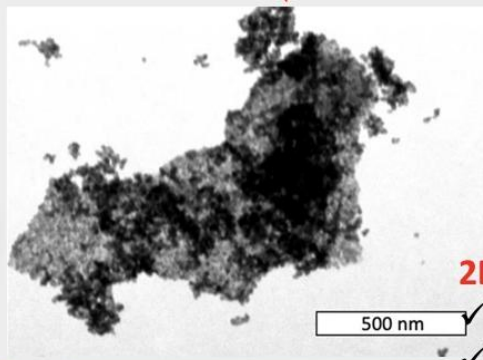
- ✓ Allows Li-ions
- ✓ Block polysulfides

Nano scale spacer

- ✓ Regulated space
- ✓ Confined Sulfur host

2D orientation

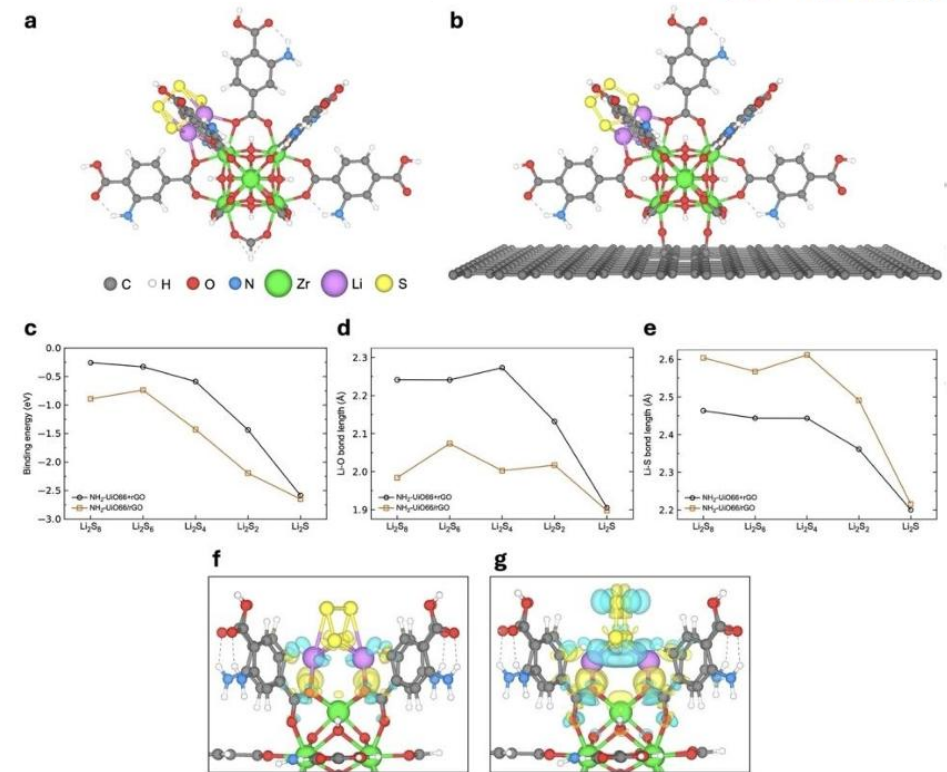
- ✓ Conductivity
- ✓ Immobilize PLS



Physical mixing of MOF with conductive rGO

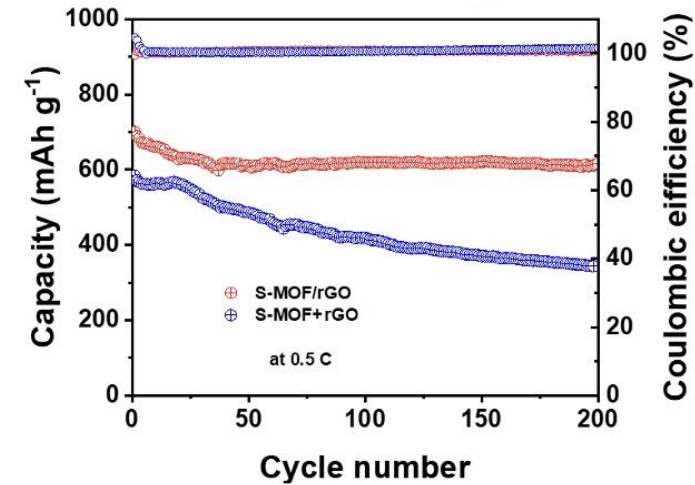
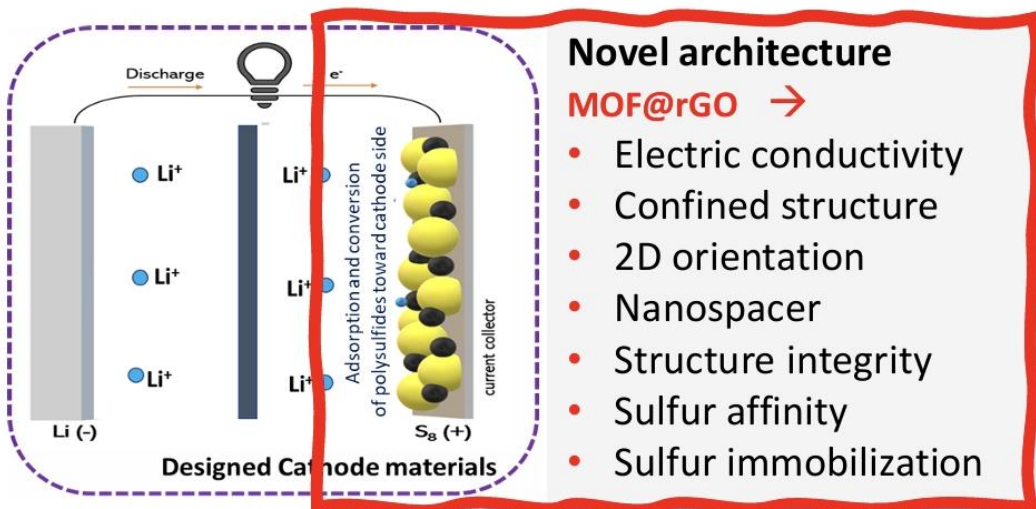
In situ growing MOF on basal planes of 2-D rGO

* rGO- reduced graphene oxide

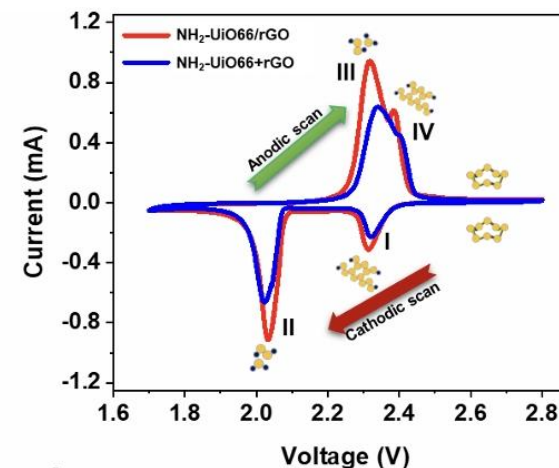


→ Representative **DFT calculated** adsorption structures of Li₂S₄ on NH₂-UiO66+rGO (a) and NH₂-UiO66@rGO (b). Calculated binding energies (c), Li-O bond lengths (d), and Li-S bond lengths (e) for Li₂S_n ($n = 1, 2, 4, 6, 8$). Differential charge density surrounding adsorbed Li₂S₄ on NH₂-UiO66 (f) and NH₂-UiO66/C (g). Yellow and blue represent increase or loss in electronic charge, with iso surfaces set to 0.002 Å⁻¹.

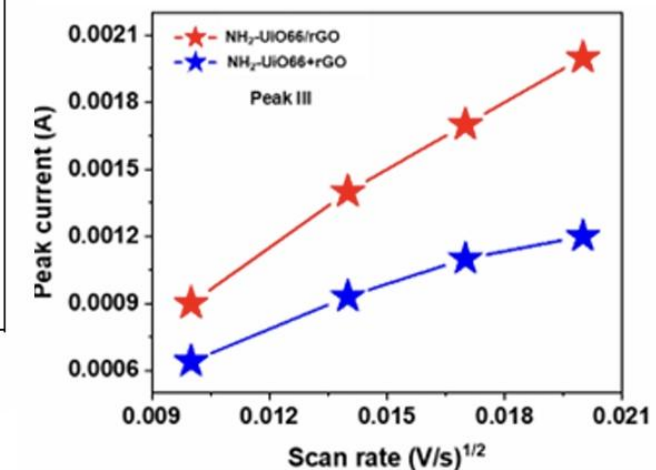
MOF@rGO-based S cathode: Comparison of MOF+rGO vs. MOF@rGO



Up figure: The cyclic performance was measured at a current density of 0.5 C. The charge/discharge voltage range was 1.6-2.8 V

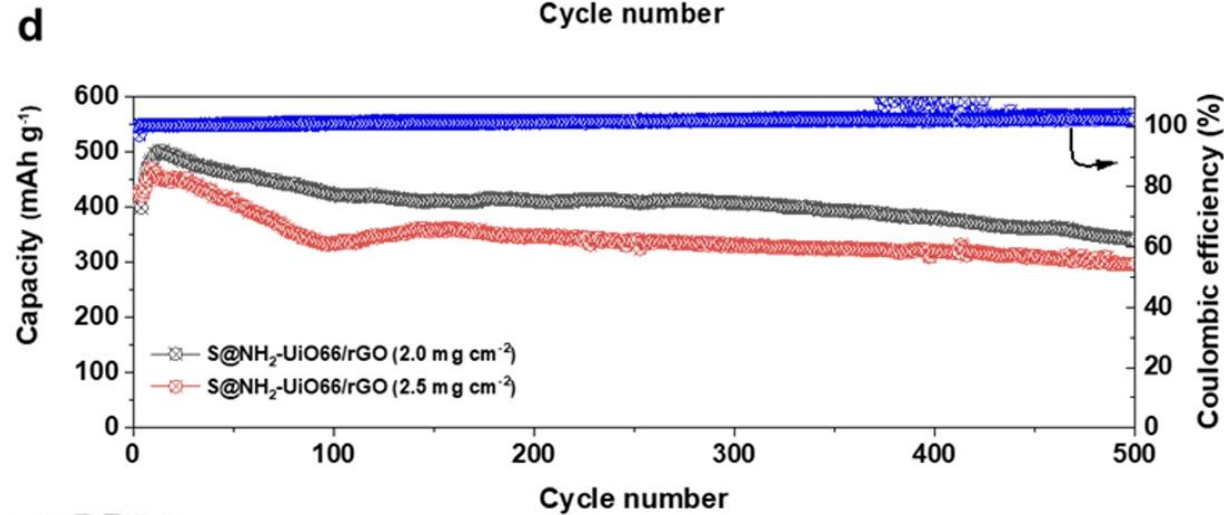
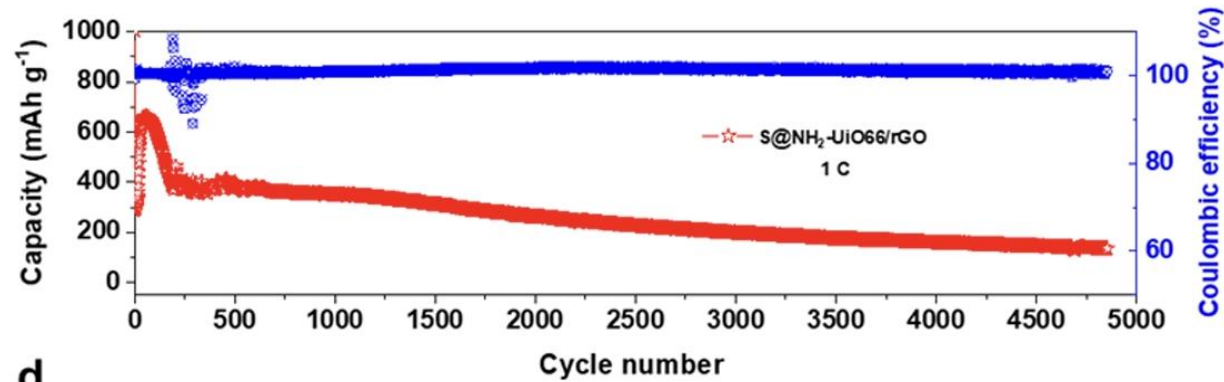


Left: Cyclic voltammetry (CV) profiles.
Right: Li⁺ diffusion behavior analysis of anodic peaks

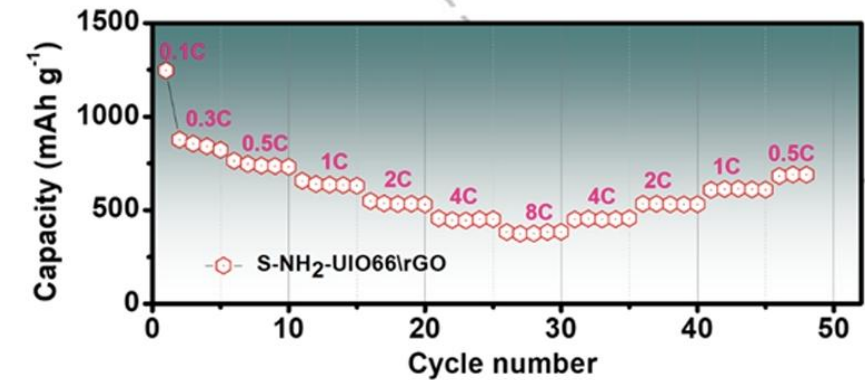


MOF@rGO-based cathodes for Li-S Batteries: performances

- ✓ Ultra long (4800) cyclic performance of the S@NH₂-UiO66/rGO cathode at 1 C (up)
- ✓ Cyclic performance of S@NH₂-UiO66/rGO cathode at high areal loading at 5C (down)



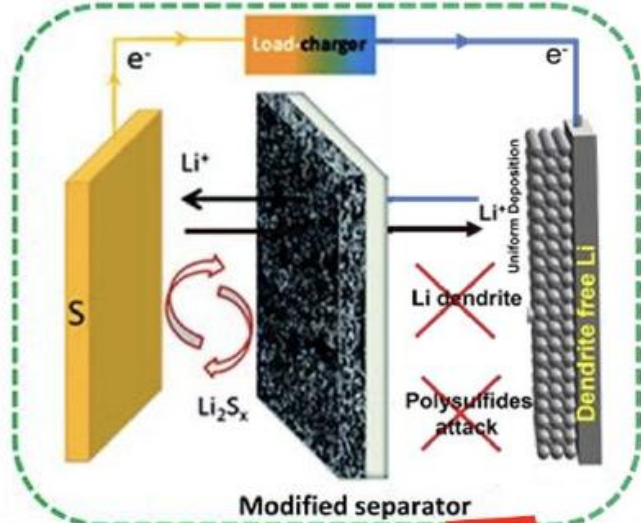
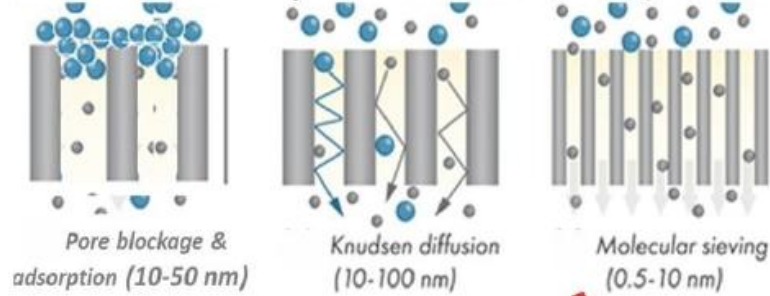
- ✓ Li-S battery with S-MOF@rGO cathode at different current densities



C-Rate	Initial capacity (mAh g ⁻¹)	Reversible capacity (mAh g ⁻¹)
0.1	1246	
0.3	870	
0.5	764	691
1	675	613
2	594	533
4	455	450
8	384	

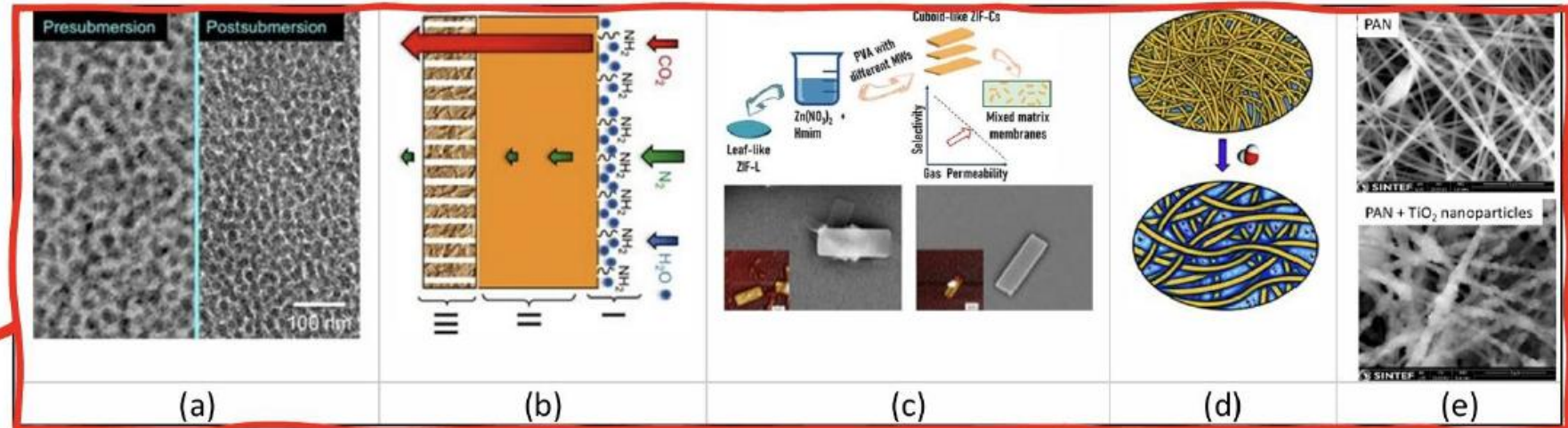
3S Battery: separator design concepts

Membrane transport mechanisms (channels)

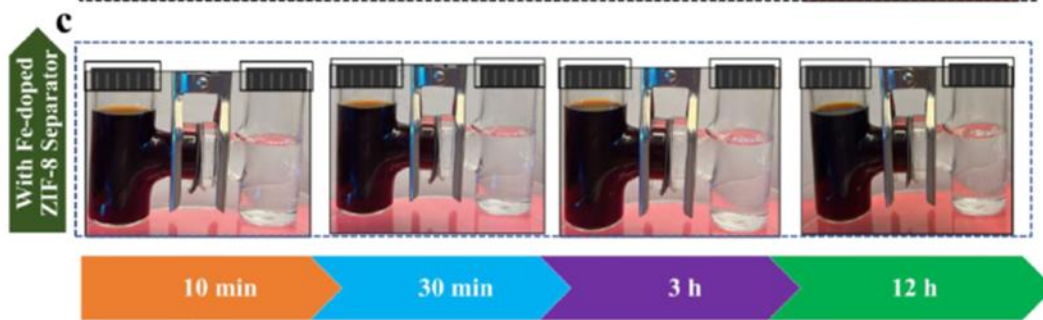
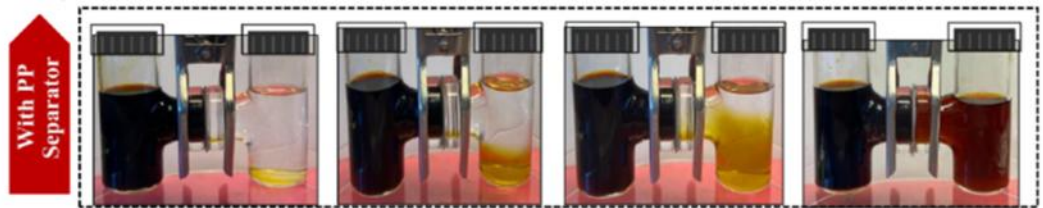
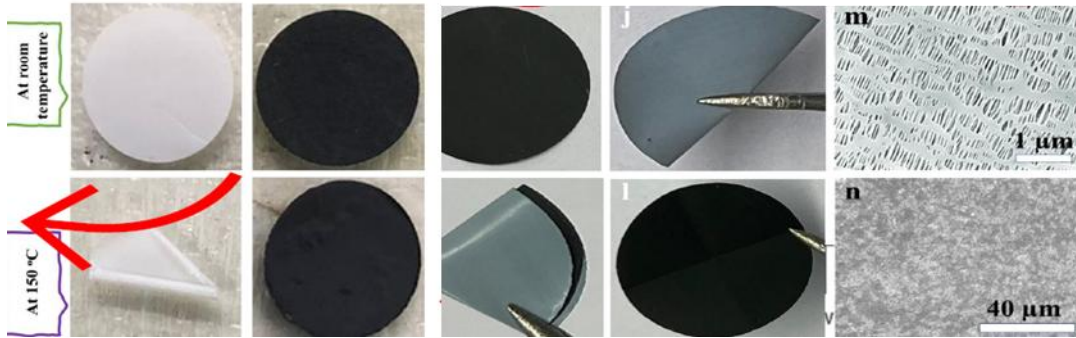


Proposed approaches in the 3S Battery project

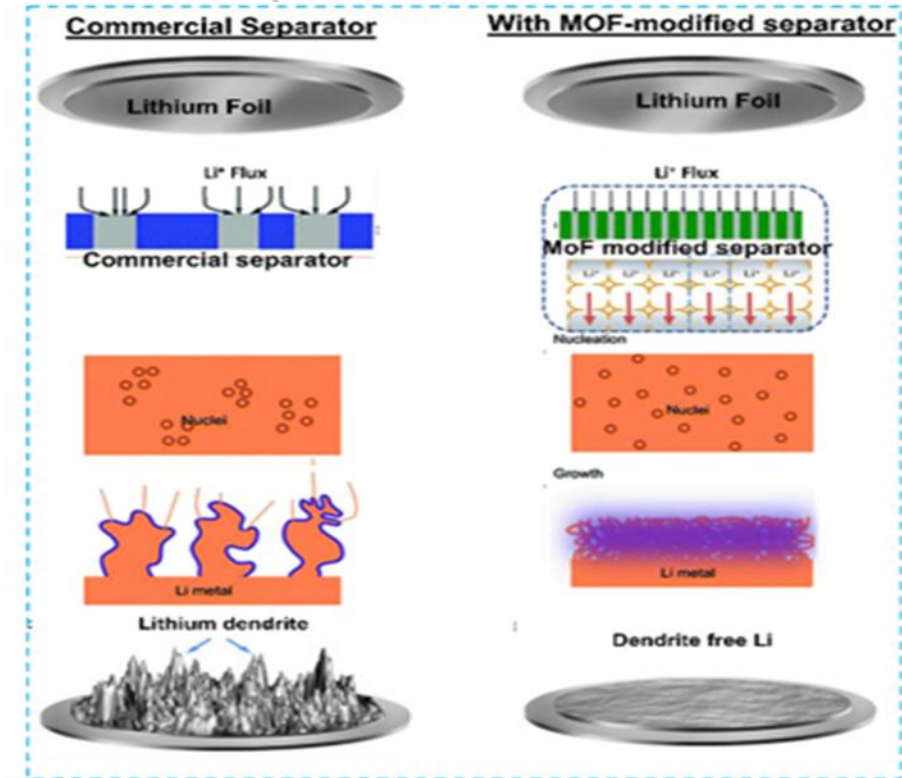
- **Multifunctional nanomaterials (MOF, COF, etc)** by performance-structure design approaches
- Specifically defined **ultrathin film morphology** and functionalities
- **Janus membranes and hybrid membranes**
- **Electrospinning nonwoven structures** with optimized hierarchical pore structure and properties.



An example: Performances of **bimetallic MOF** separator for Li-S batteries



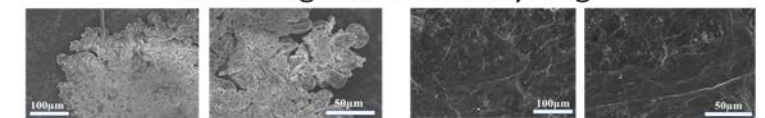
d



Surface morphologies of the Li plate after 1000 cycles

e

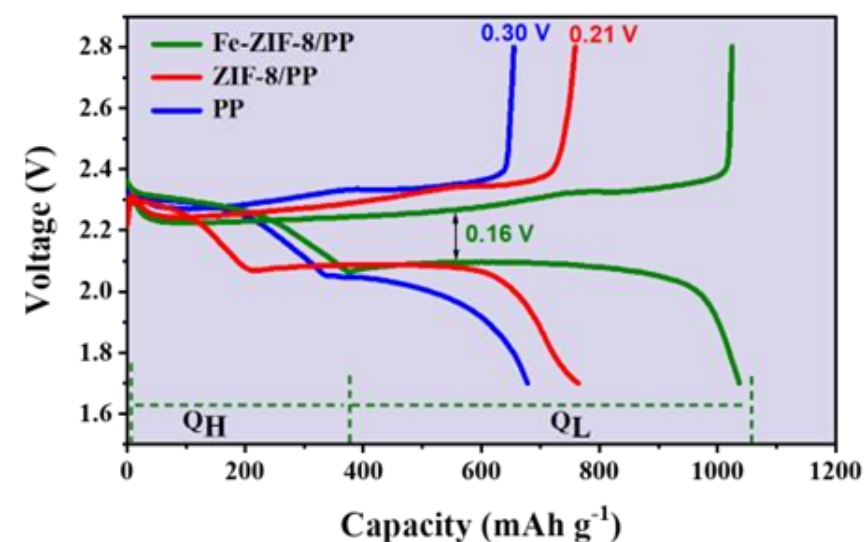
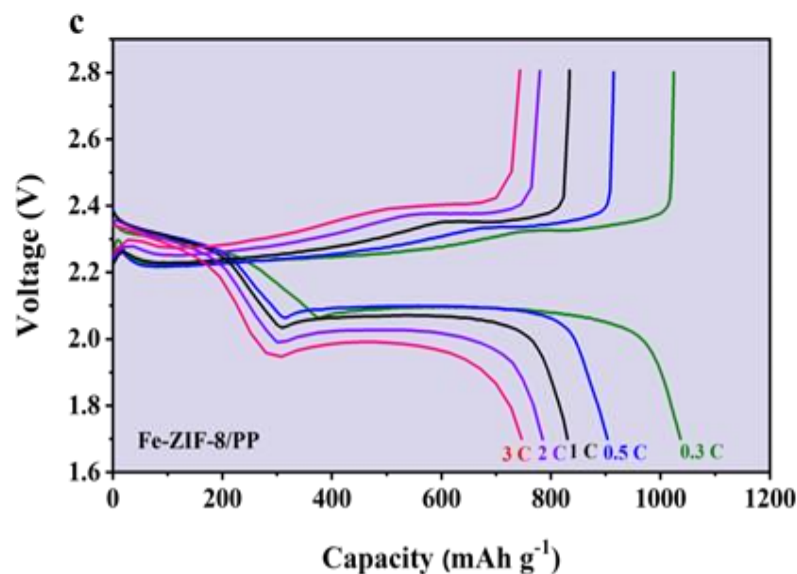
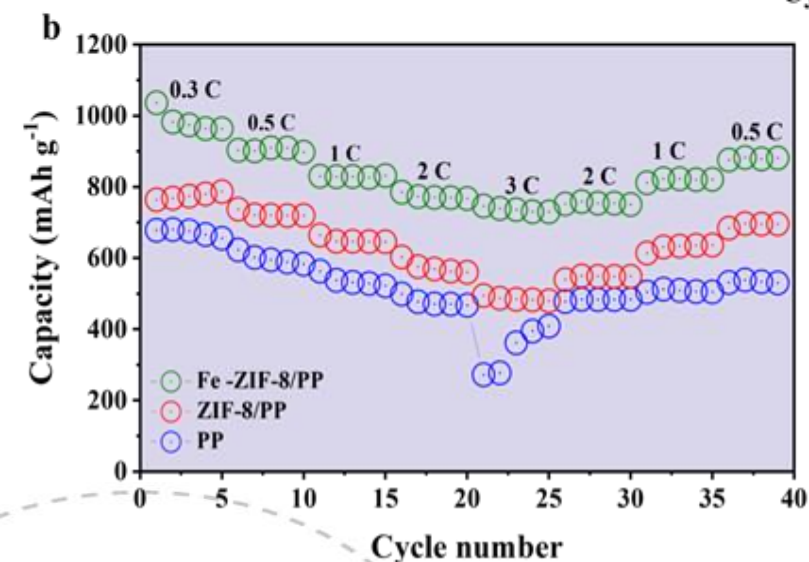
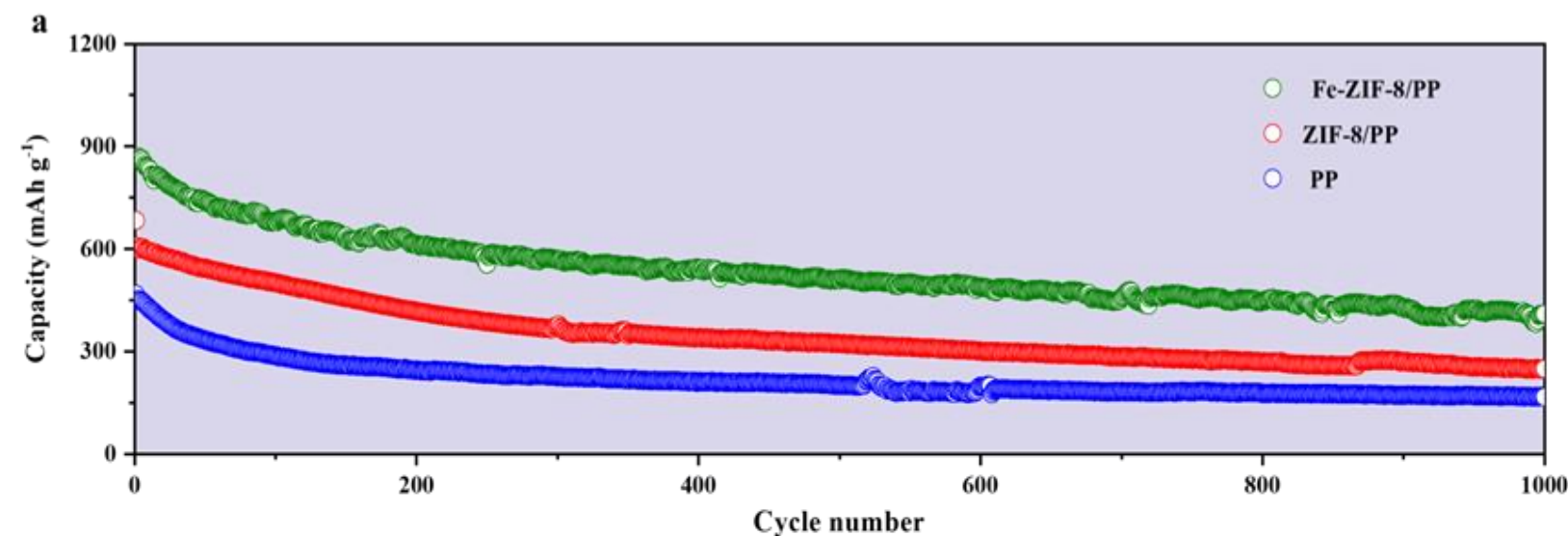
SEM images of Li After cycling



With PP separator

With a modified PP separator

Performances of bimetallic MOF separator for Li-S batteries



- a) Long-term cycling performance of the Li-S batteries at 0.5 C
- b) The rate capability at different current densities /C-rates
- c) Discharge and charge profiles at different C-rates for Li-S batteries with Fe-ZIF-8/PP separator
- d) Comparison of separators at 3C

Thank you!

