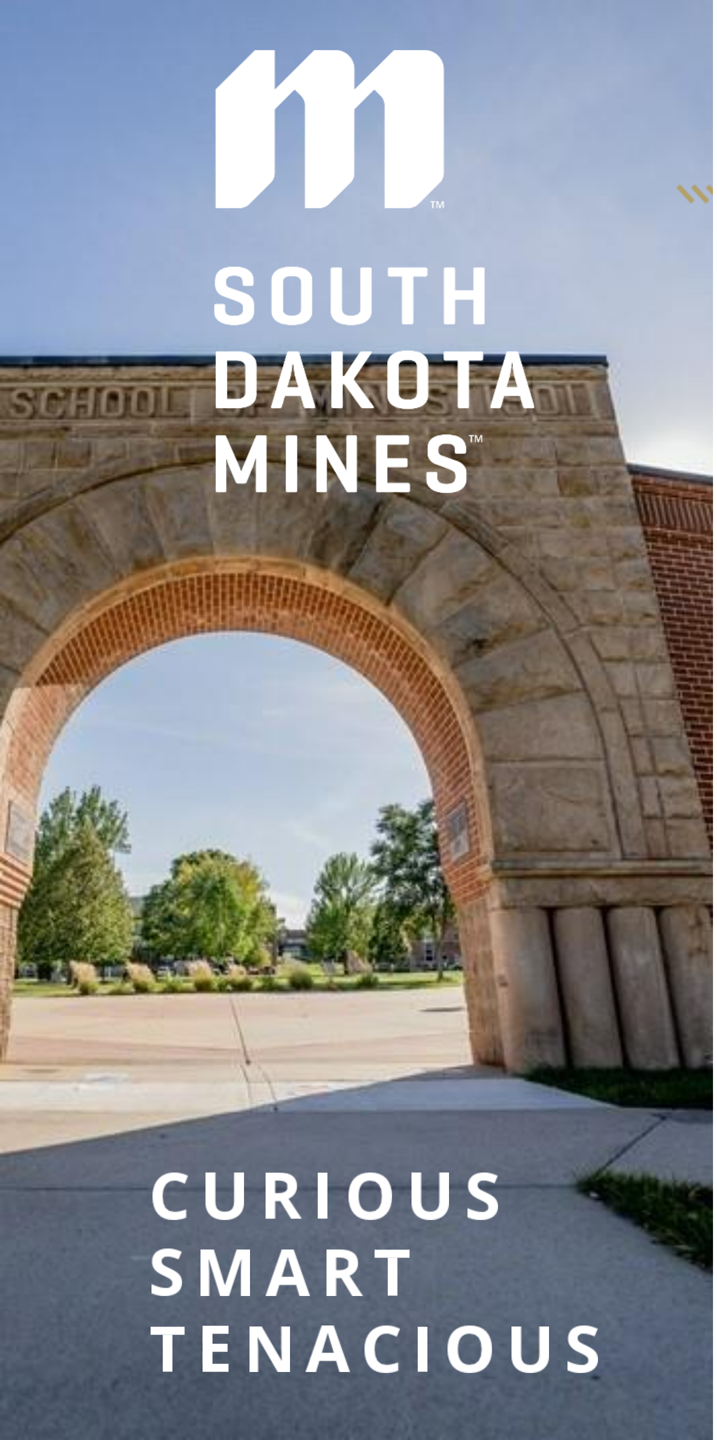

Scalable, High Energy Density Lithium-Sulfur Batteries (SD-LSB)

NASA Battery Workshop
Nov 16, 2022, Huntsville, AL

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NASA's energy storage needs for future space missions

- NASA JPL Whitepaper "Energy Storage Technologies for Planetary Science and Astrobiology Missions". May 01, 2021*

Table 3: Performance Characteristics of Emerging Rechargeable Battery Technologies

Technology	Projected Performance (75% of Cell level)				Challenges	Key Players	TRL
	Wh/kg	Wh/l	Cycle Life	Temp			
Li-S with Liquid Ely'te	325	600	200	-20 to +50	Sulfur shuttle, Li dendrites, Safety?	Oxis Energy, Sion Power ,	3

325 Wh/kg (battery level) → 433 Wh/kg (cell level)

* Bugga, R.; Brandon, E.; Darcy, E.; Ewell, R.; Faguay, P.; et al. "Energy Storage Technologies for Planetary Science and Astrobiology Missions". May 01, 2021.

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Li-S battery advantages

- **High theoretical specific capacity / energy**

  S half redox reaction:

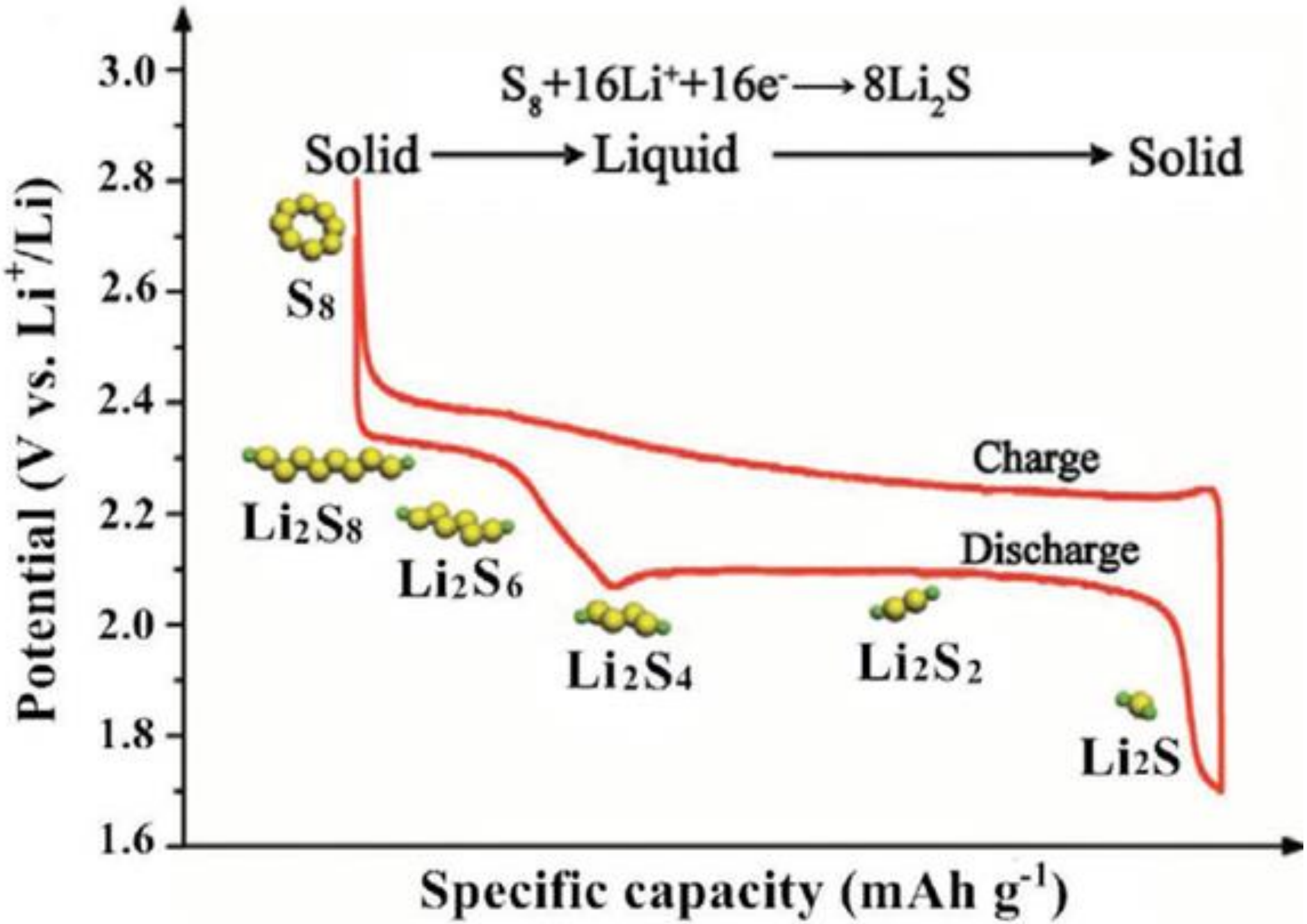
  $S_8 + 16Li^+ + 16e^- \leftrightarrow 8Li_2S$ or

  $S + 2Li^+ + 2e^- \leftrightarrow Li_2S$ (Li_2S = lithium sulfide)

  S theoretical specific capacity **1,675 mAh/g**

  Li-S battery theoretical specific energy ~ 2,500 Wh/kg
- **Naturally abundant**
- **Low cost**
- **Environmentally friendly**

Li-S battery challenges

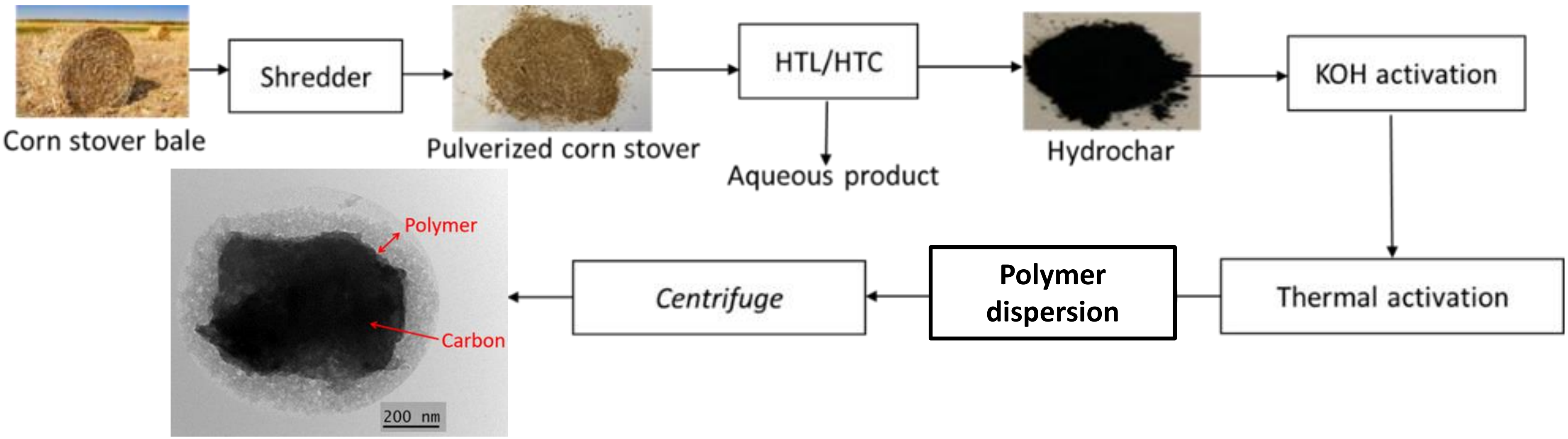


- S cathode and Li form a series of intermediates (**Li_2S_n** n>1) before the final product (**Li_2S**)

Li-S battery challenges

- **Dissolution of high-order Li polysulfides (LPS), Li_2S_n (4 ≤ n ≤ 8)**
  - Diffusion of LPS anions (S_n^{2-}) through the separator to the negative Li anode can cause
- **LPS shuttle phenomenon during charge**
  - High order LPS diffuses to the negative electrode and reacts with Li anode to form low order LPS
  - Low order LPS diffuses back to the positive electrode to be oxidized to form high order LPS
- **Poor electronic conductivity of S and low order LPS**
  - S is 5×10^{-30} S/cm at 25°C; (compare Cu 6×10^{7} S/cm)
  - Low order LPS (Li_2S_2, Li_2S) are insulating in nature
- **Sulfur electrode volume change**
  - ~76% volume change during cycling → loss of particle contact
- **Use of metallic Li anode**
  - Dendrite formation → safety concerns

Nanolayer polymer modified carbon (NPC)



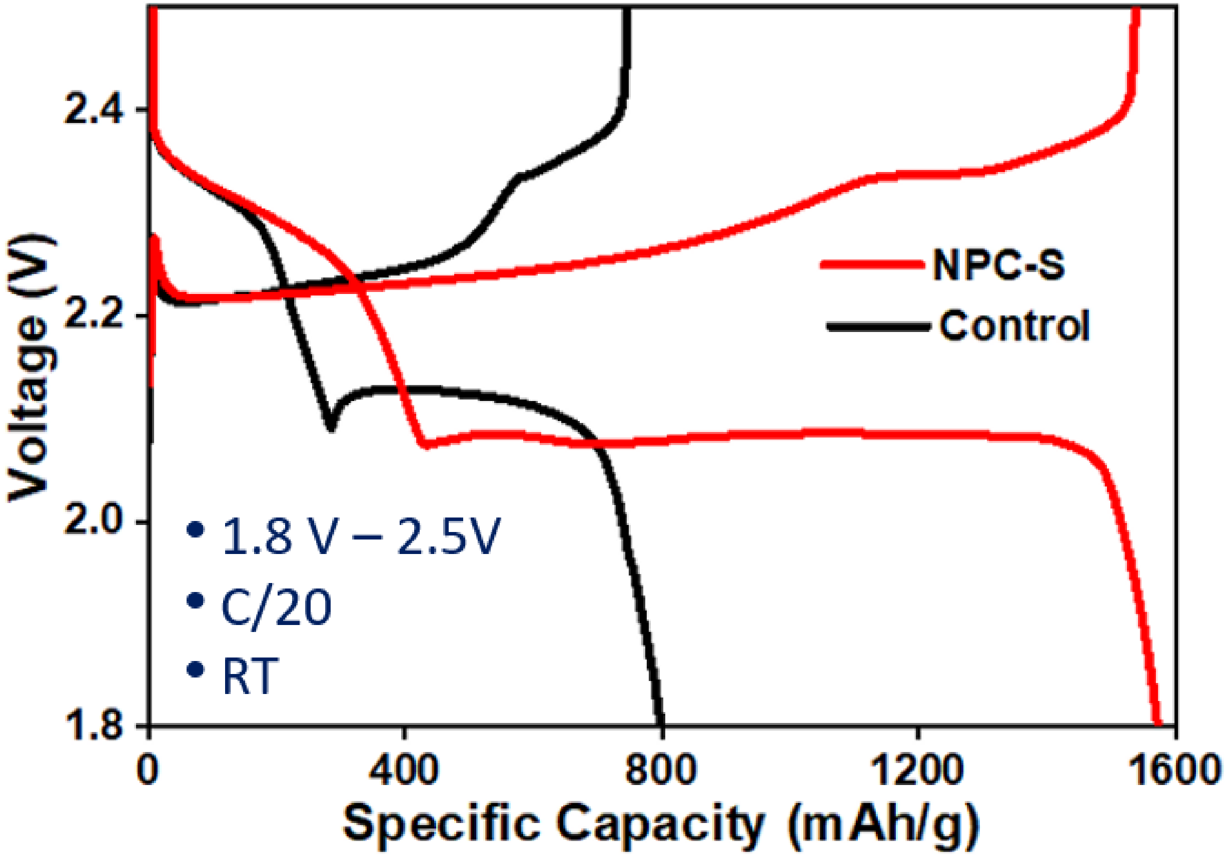
NPC

- Renewable biomass corn stover starting material
- Final product: **NPC**.

Li-S battery preparation

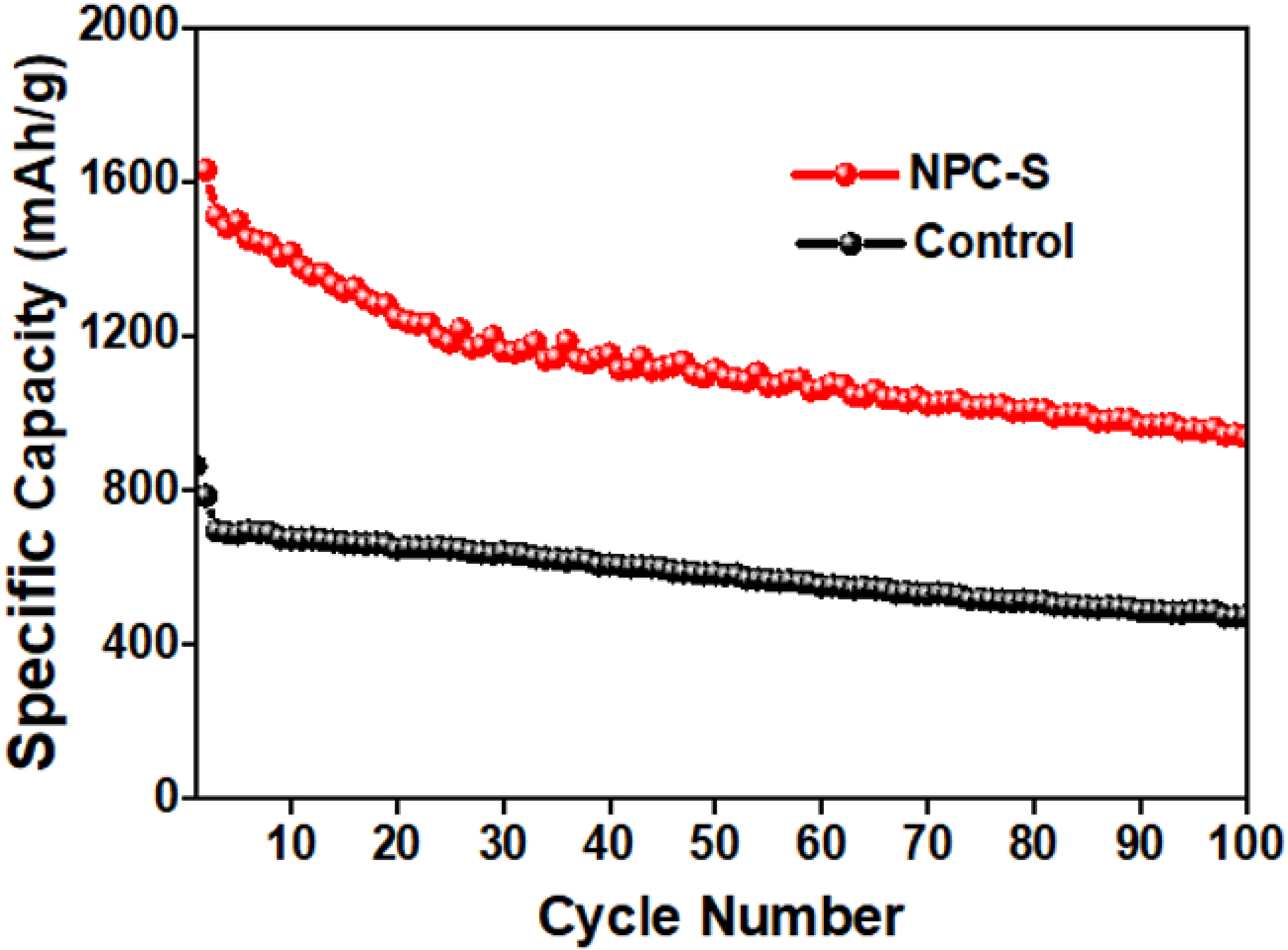
- NPC modified sulfur electrodes: **NPC-S**.
- Baseline sulfur electrodes: Control
- Li anodes
- Electrolyte: LiTFSI in DOL/DME
- Polyolefin separators
- CR2032 coin-type cell hardware

Specific capacity of Li-S cells



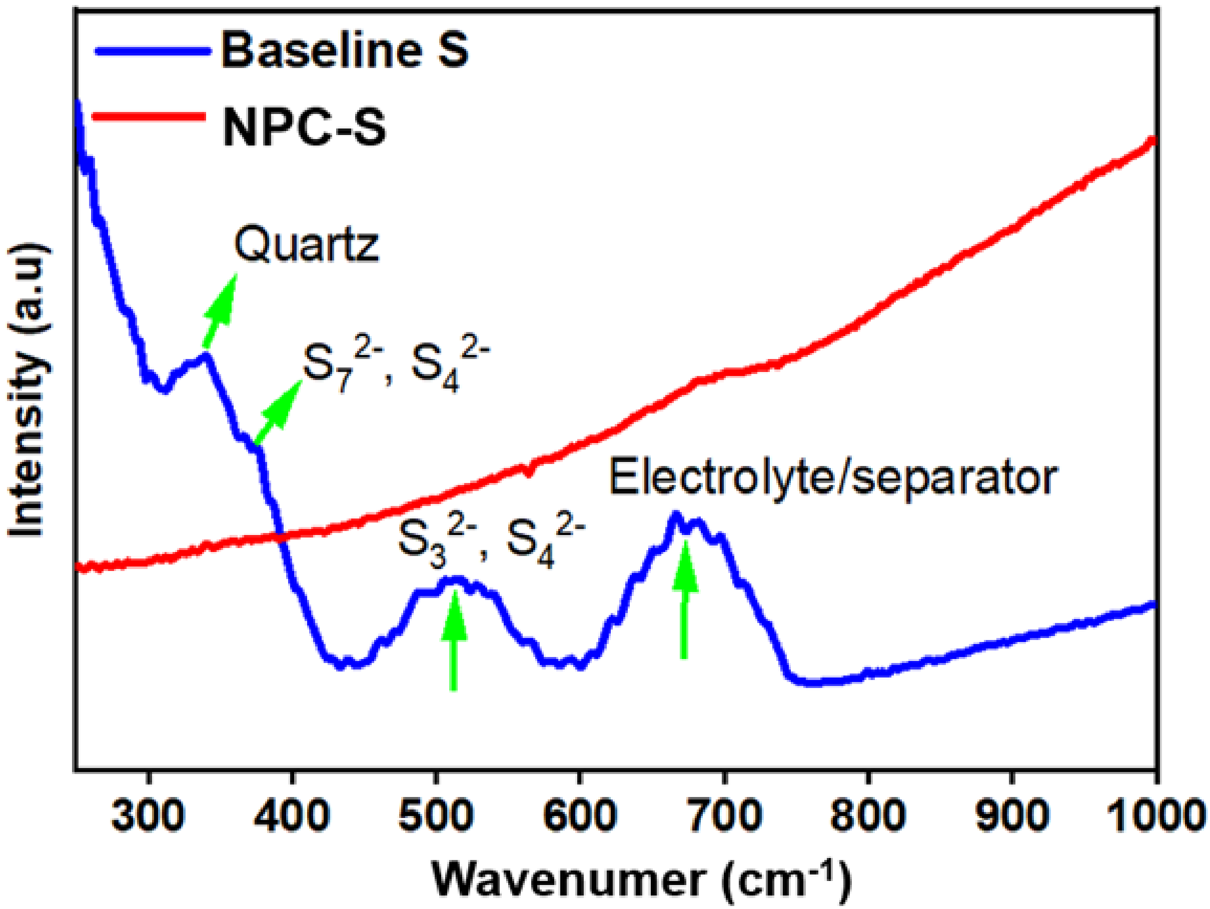
- NPC-S cell delivered discharge specific capacity ~1,600 mAh/g which approaches the theoretical value of 1,672 mAh/g
- The control cell delivered only 800 mAh/g due to adverse effect of PS formation resulting in loss of active sulfur

Cycle life of Li-S cells



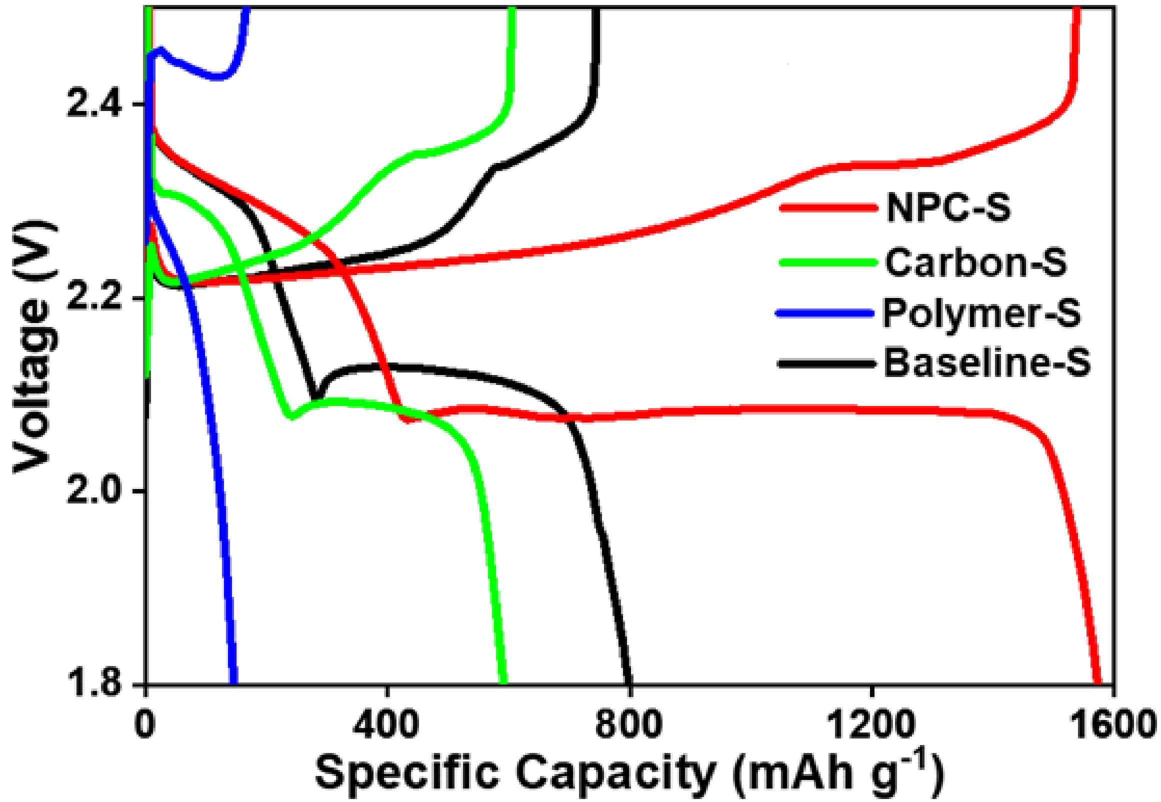
- The NPC-S based cell delivered twice the specific capacity than the baseline-S cell (940 mAh/g vs. 470 mAh/g) after 100 cycles

In-situ Raman of Li-S cells



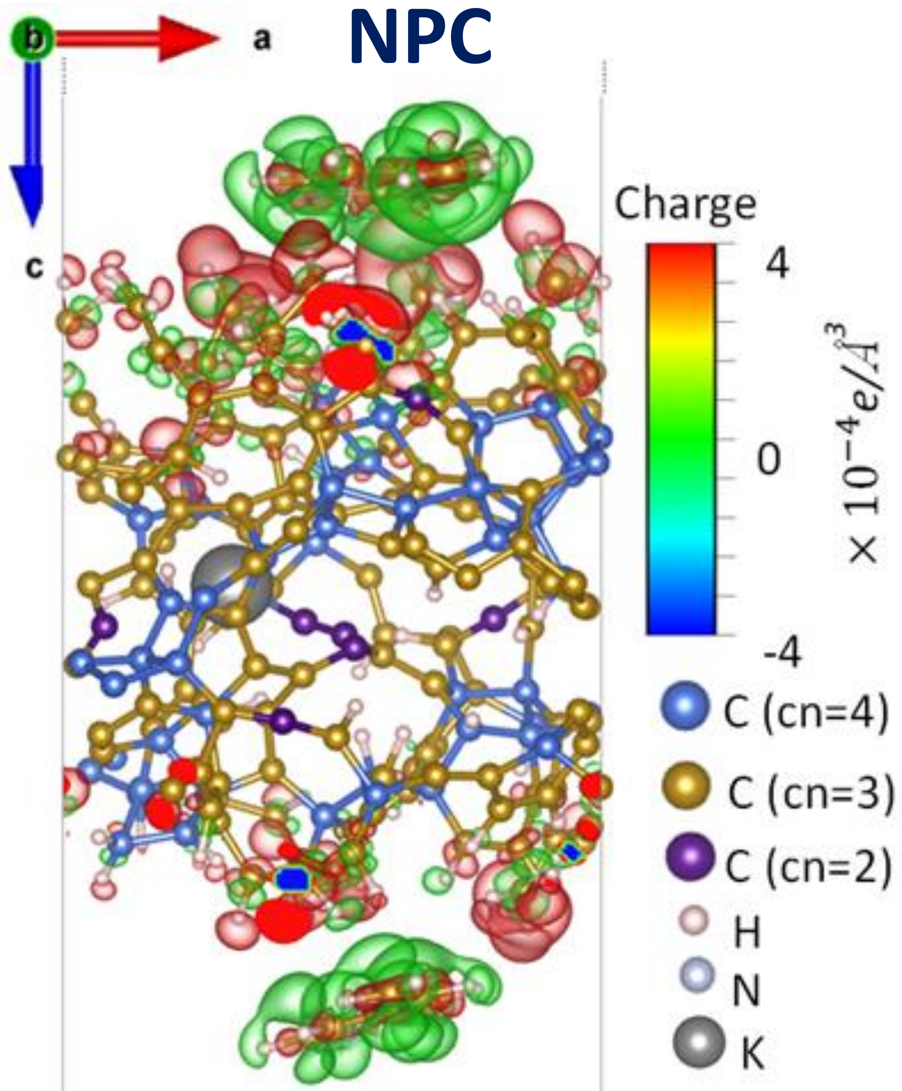
- The baseline-S showed characteristic PS peaks due to dissolution of PS species into the electrolyte
- The NPC-S showed no PS peaks (no PS dissolution into the electrolyte)

Comparative study



- The Carbon-S and Polymer-S cells delivered significantly lower discharge specific capacities, 580 mAh/g and 140 mAh/g, respectively, than 1,600 mAh/g of the NPC-S cell.
- No or inadequate PS trapping capability and large charge transfer interfacial impedance led to the low discharge specific capacities of the Carbon-S and Polymer-S cells

Molecular dynamics simulation



- Interfacial charge distribution:
  red: electron gain
  green: electron loss
- Accumulation of opposite charges on NPC leads to the formation of surface dipoles.
- MD simulation suggests NPC's PS trapping capability arises from dipole-dipole interactions

Conclusions

- A new type of PS-trapping material, NPC, was studied
- NPC-S based Li-S cells demonstrated near theoretical discharge specific capacities
- Our novel approach is simple, low-cost, and economically scalable for large-scale commercialization
- SD-LSB holds promise to address NASA battery energy storage needs for future space missions

Acknowledgement

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