

## ABSTRACT

Lithium-organic batteries offer a sustainable alternative to lithium-ion batteries, with porous organic polymers (POPs) emerging as promising organic electrodes. Inspired by the excellent electrochemical performance of naturally occurring phenolic compounds, we explore using gallic acid and ellagic acid to couple with 2,6-diamino anthraquinone (2,6-DAAQ), yielding organic polymers. Results indicate that AQ-ellagic acid polymers exhibit superior battery performance compared to AQ-gallic acid, which exhibits 582 mA h g<sup>-1</sup> for ellagic acid and 474 mA h g<sup>-1</sup> for gallic acid at 100 mA g<sup>-1</sup>. Additionally, a cost analysis and sustainability assessment based on the green chemistry principles of natural phenolic compounds as organic electrode materials will be discussed. This study highlights the potential of biomass-derived phenolic compounds as coupling monomers for sustainable organic electrode materials in eco-friendly lithium-organic batteries.

## INTRODUCTION

- Lithium-ion batteries** are widely used due to their lightweight and high energy capacity. However, concerns over the limited availability of resources and the environmental impact of hazardous waste from batteries highlight the need for more sustainable alternatives.
- Lithium-organic batteries** have emerged as a promising solution, utilizing abundant, non-toxic materials for electrodes and offering high theoretical capacity.
- Our study explores using 2,6-DAAQ in azo coupling polymerization with gallic acid and ellagic acid as organic electrode materials for lithium-organic batteries. These materials were chosen for their sustainability, environmental friendliness, and potential to improve energy storage performance.

### Selected References

- Chem. Eng. J. **2023**, 466, 143090 (<https://doi.org/10.1016/j.cej.2023.143090>)
- ChemElectroChem. **2019**, 6, 4765–4772 (<https://doi.org/10.1002/celec.201901064>)
- ACS Appl. Energy Mater. **2023**, 6, 7826–7836 (<https://doi.org/10.1021/acsaem.3c00586>)

## RESEARCH OBJECTIVES

- To investigate the use of natural phenolic compounds to synthesize organic polymer for lithium-organic batteries.
- To study cost analysis and sustainability assessment based on green chemistry of using natural compounds as organic electrode materials in lithium-organic battery.

## RESEARCH METHODOLOGY

### 1. Synthesis and Characterizations

- FT-IR
- Solid-state <sup>13</sup>C NMR
- Elemental analysis
- N<sub>2</sub> sorption study
- TGA

### 2. Battery performance testing

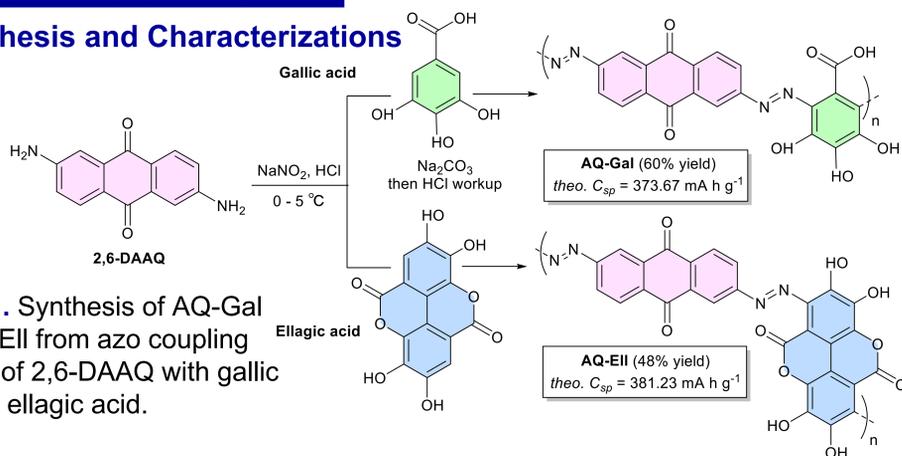
- Coin cell assembly
- Galvanostatic charge/discharge
- Rate performance

### 3. Cost analysis and sustainability assessment

- E-factor
- Atom economy

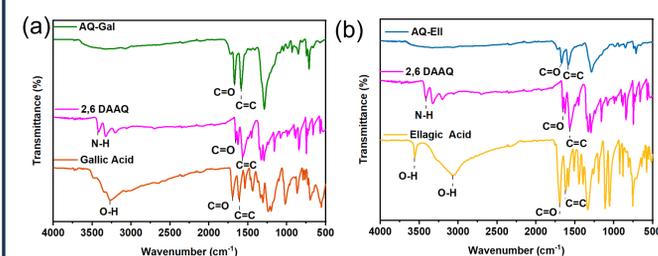
## RESULTS AND DISCUSSION

### 1. Synthesis and Characterizations

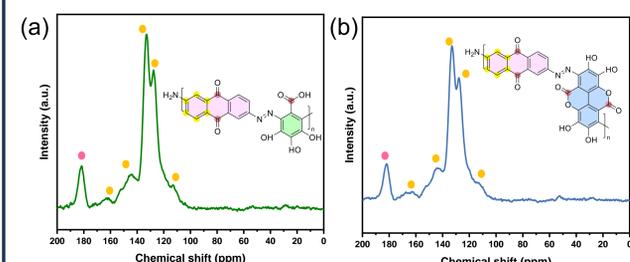


**Figure 1.** Synthesis of AQ-Gal and AQ-Ell from azo coupling reaction of 2,6-DAAQ with gallic acid and ellagic acid.

- 2,6-DAAQ was successfully coupled with gallic acid and ellagic acid via the azo coupling reaction yielding polymers AQ-Gal and AQ-Ell in 60% and 48% yields.



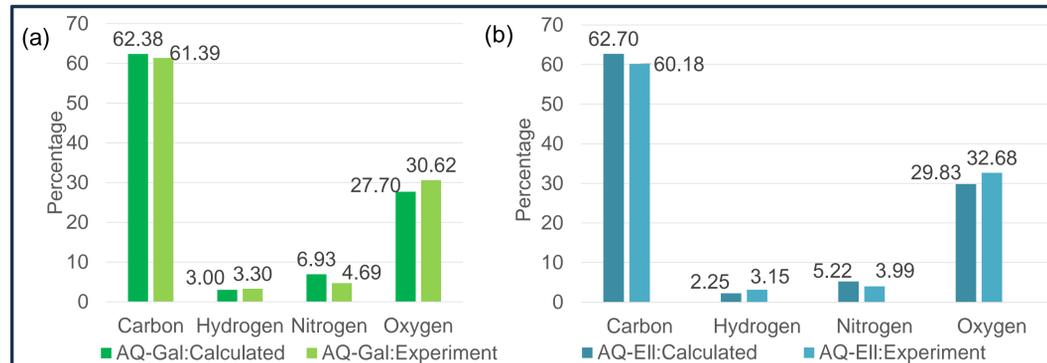
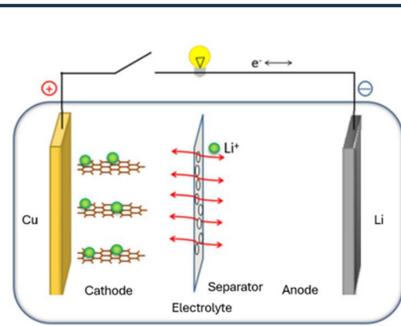
**Figure 2.** FT-IR spectra of (a) AQ-Gal and (b) AQ-Ell.



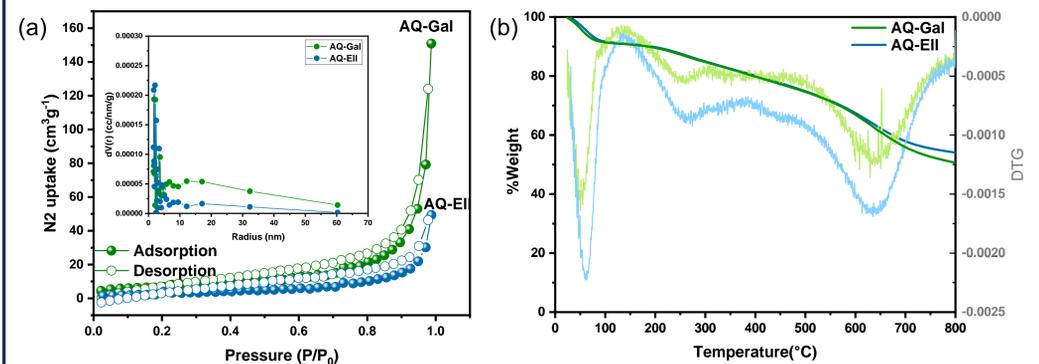
**Figure 3.** Solid-state <sup>13</sup>C NMR spectra of (a) AQ-Gal and (b) AQ-Ell.

- FT-IR analysis confirmed the key functional groups
- The appearance of stretching at 1674 cm<sup>-1</sup> (C=O of AQ) with the disappearance of N-H stretching.

- The <sup>13</sup>C NMR spectra confirmed the structural integrity of the polymers.
- The chemical shifts at 113–162 ppm (aromatic carbons), 181 ppm (C=O of AQ, ester and carboxylic acid) functional groups.



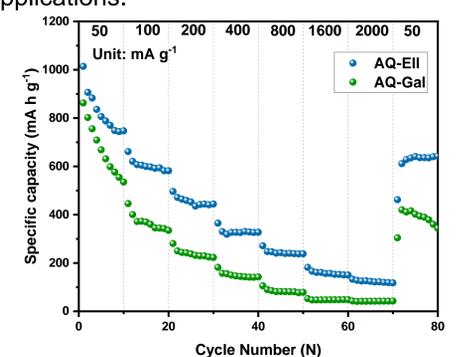
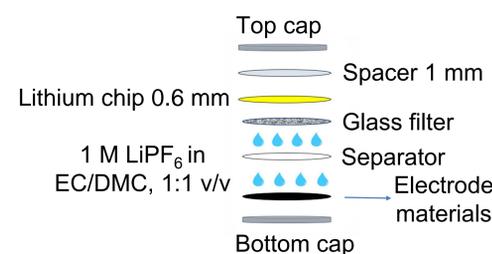
**Figure 4.** Elemental analysis of (a) AQ-Gal and (b) AQ-Ell.



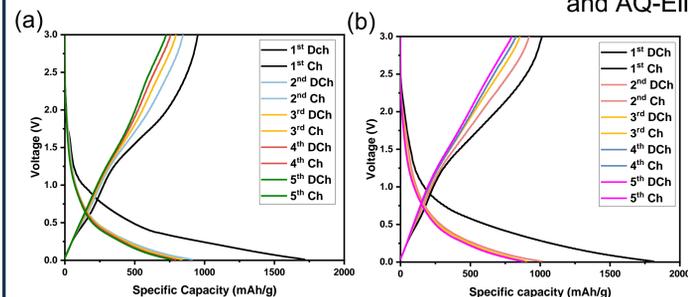
**Figure 5.** (a) N<sub>2</sub> sorption isotherms and (b) TGA profile of AQ-Gal and AQ-Ell.

- The N<sub>2</sub> sorption isotherms of AQ-Gal and AQ-Ell exhibit type IV (mesoporous), BET Surface Area & Porosity: AQ-Gal (30.225 m<sup>2</sup>/g, 7.95 nm pore width) vs. AQ-Ell (8.123 m<sup>2</sup>/g, 7.97 nm pore width).
- TGA results show comparable thermal stability for AQ-Gal and AQ-Ell, initial weight loss below 100°C due to moisture/solvent, with mass stability maintained up to 250°C, their suitability for high-temperature applications.

## 2. Battery Performance Testing



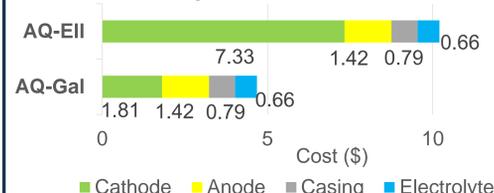
**Figure 6.** Rate performance of AQ-Gal and AQ-Ell at various current densities.



**Figure 7.** GCD profiles of (a) AQ-Gal and (b) AQ-Ell

- AQ-Ell demonstrated higher discharge capacity and superior rate performance than AQ-Gal due to its structure providing more redox-active sites for lithium-ion accommodation.

## 3. Cost Analysis and Sustainability Assessment



**Figure 8.** Cost analysis of AQ-Gal and AQ-Ell

**Table 1.** E-factor and atom economy of AQ-Gal and AQ-Ell

	E-factor	Atom Economy
AQ-Gal	8.00	67%
AQ-Ell	8.70	71%

## CONCLUSION

- AQ-Gal and AQ-Ell were successfully synthesized and structurally confirmed through spectroscopy and elemental analysis.
- Both materials demonstrated mesoporosity and thermal stability, supporting their suitability for energy storage applications.
- AQ-Ell exhibited superior electrochemical performance due to its structure providing more redox-active sites for lithium-ion accommodation, while AQ-Gal showed greater sustainability and cost-effectiveness.