下世代鋰離子電池負極電極材料奈米結構技術

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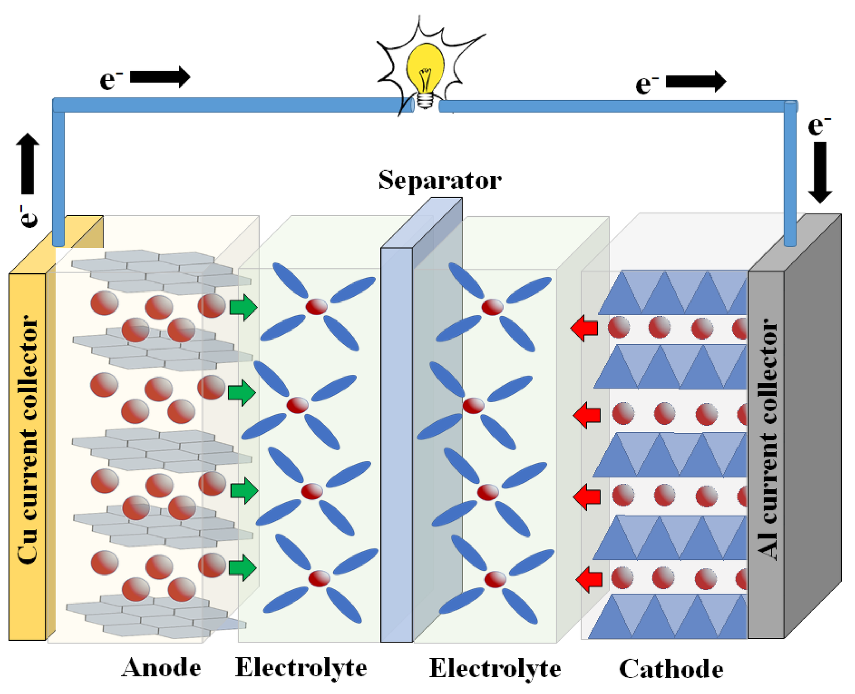
Abstract

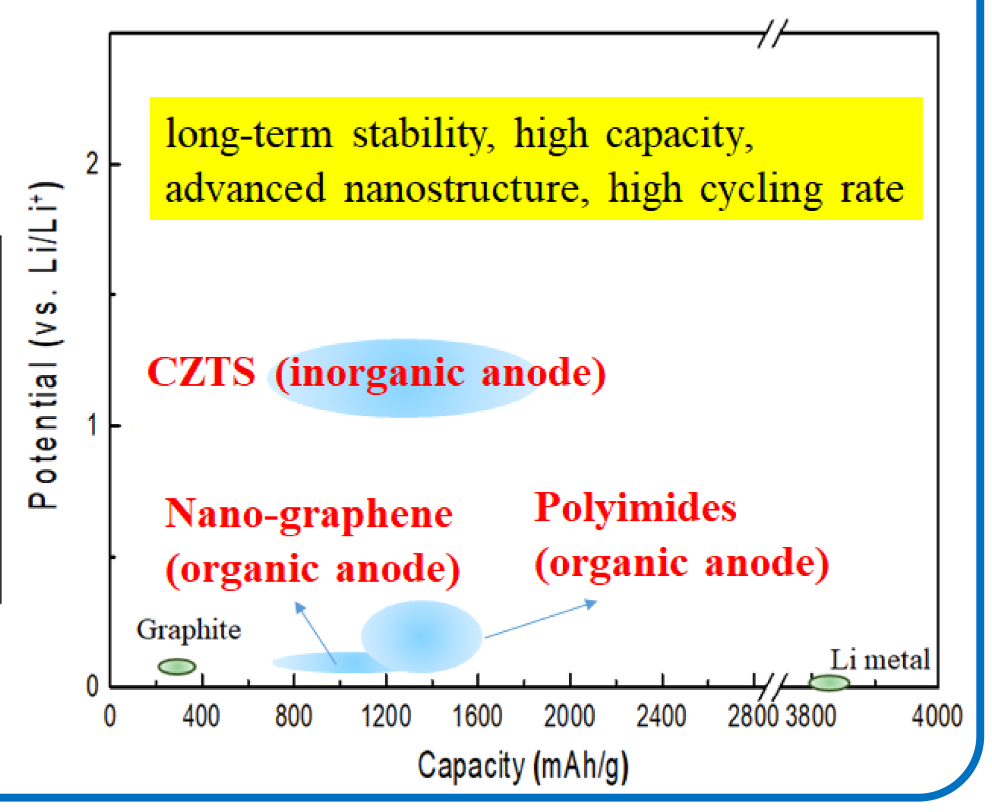
Global demand for rechargeable lithium-ion batteries has grown tremendously over the past two decades. However, lithium-ion batteries lack the higher capacity and longer life time required in electric vehicles and electricity infrastructure. In order to improve the energy density and extend the cycle life of batteries, we propose to develop the novel anode materials with advanced nanostructures. Our study includes: (a) the development of flower-like Cu_2ZnSnS_4 (CZTS) nanoflakes, polyimides and 2D nanographene anode materials. The synthesis process of these material is simple. (b) the development of machine learning platform with quantum accuracy for large scale simulation of complex battery materials. (c) the use of in situ/operando characterizations combined with theoretical calculations to gain the mechanistic insights into the eletrochemcial behavior of anode materials, (d) the cooperation with industry. The proposed organic/inorganic anode materials with higher electrochemical performance and stability will fit in conventional manufacturing processes of practical lithium-ion batteries.

Introduction

Lithium-ion batteries

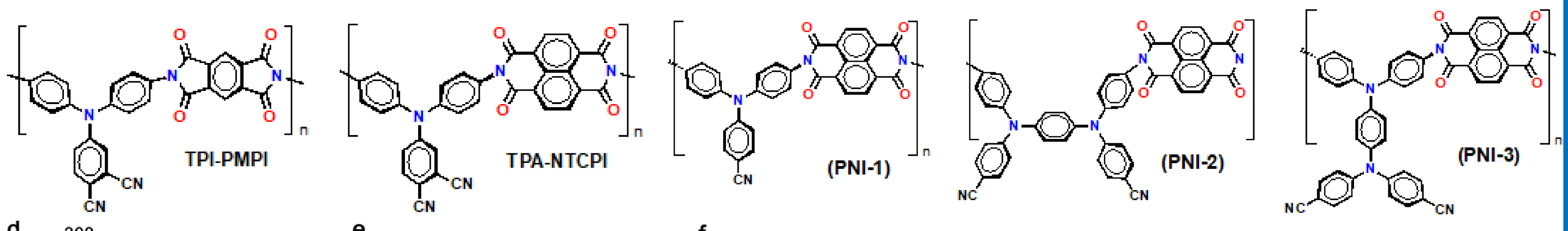


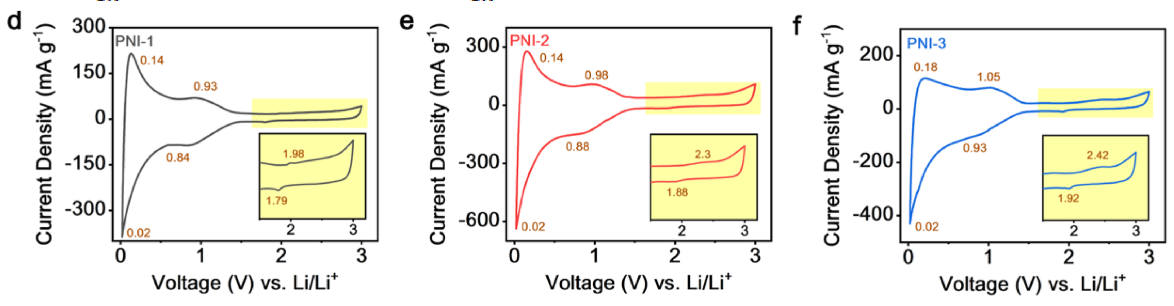
Anode materials

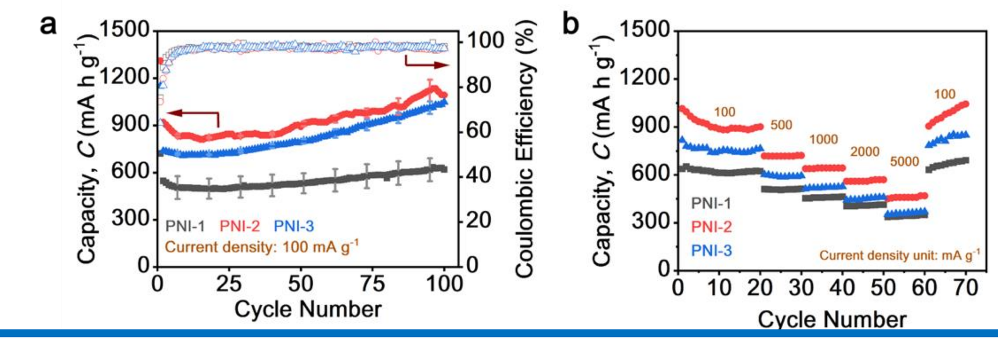


Results and Discussion

Polyimides anode materials



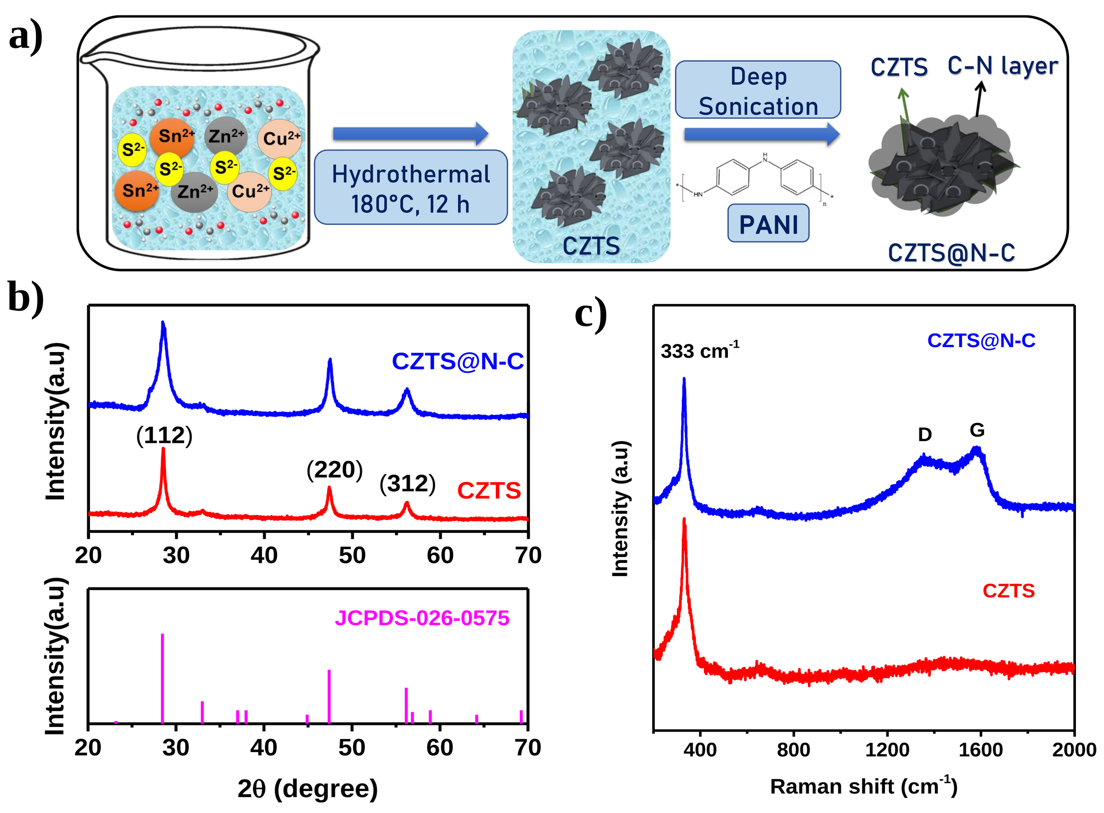




Organic anode material shows a capacity of ~1200 mAh/g after 100 cycles.

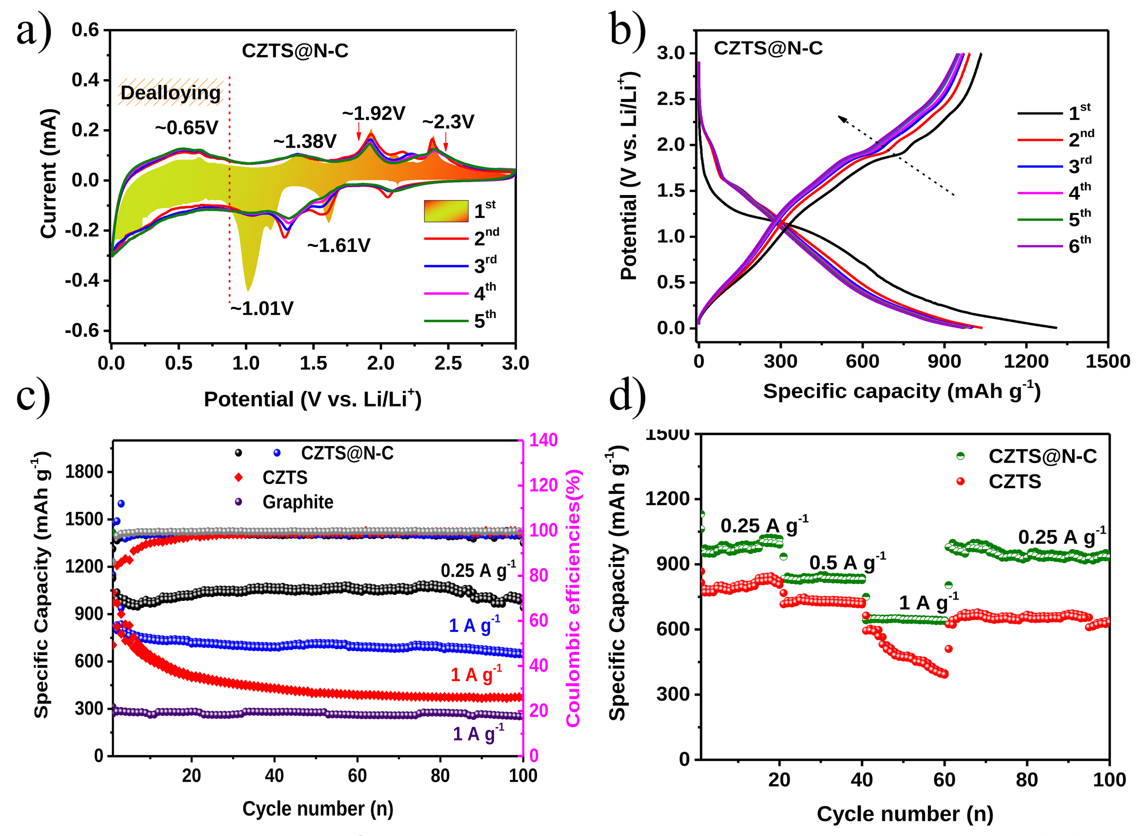
Results and Discussion

CZTS anode materials and pouch cell demonstration



(a) The synthesis process of CZTS@N-C, (b) XRD patterns and (c) Raman spectra of CZTS and CZTS@N-C.

CZTS anode materials prepared by the hydrothermal method can be modified with different ligands and coatings.

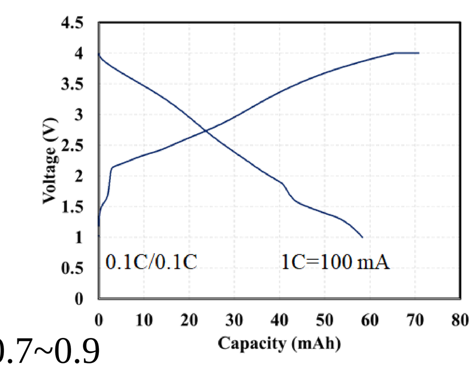


(a) CV curves of CZTS@N-C with 0.1 mV/s scan rate and (b) charge-discharge curves of CZTS@N-C at a rate of 1 A/g. (c-d) Electrochemical performance of CZTS, CZTS@N-C and graphite anode materials.

Full cell evaluation

正極	正極電容量	負極	負極電容量	平均電壓 (V)
NMC622-SC	126.24 mAh	CZTS	110.15 mAh	3.69

1.05 M LiPF6, EC/DEC-based electrolyte; A/C ratio 0.7~0.9

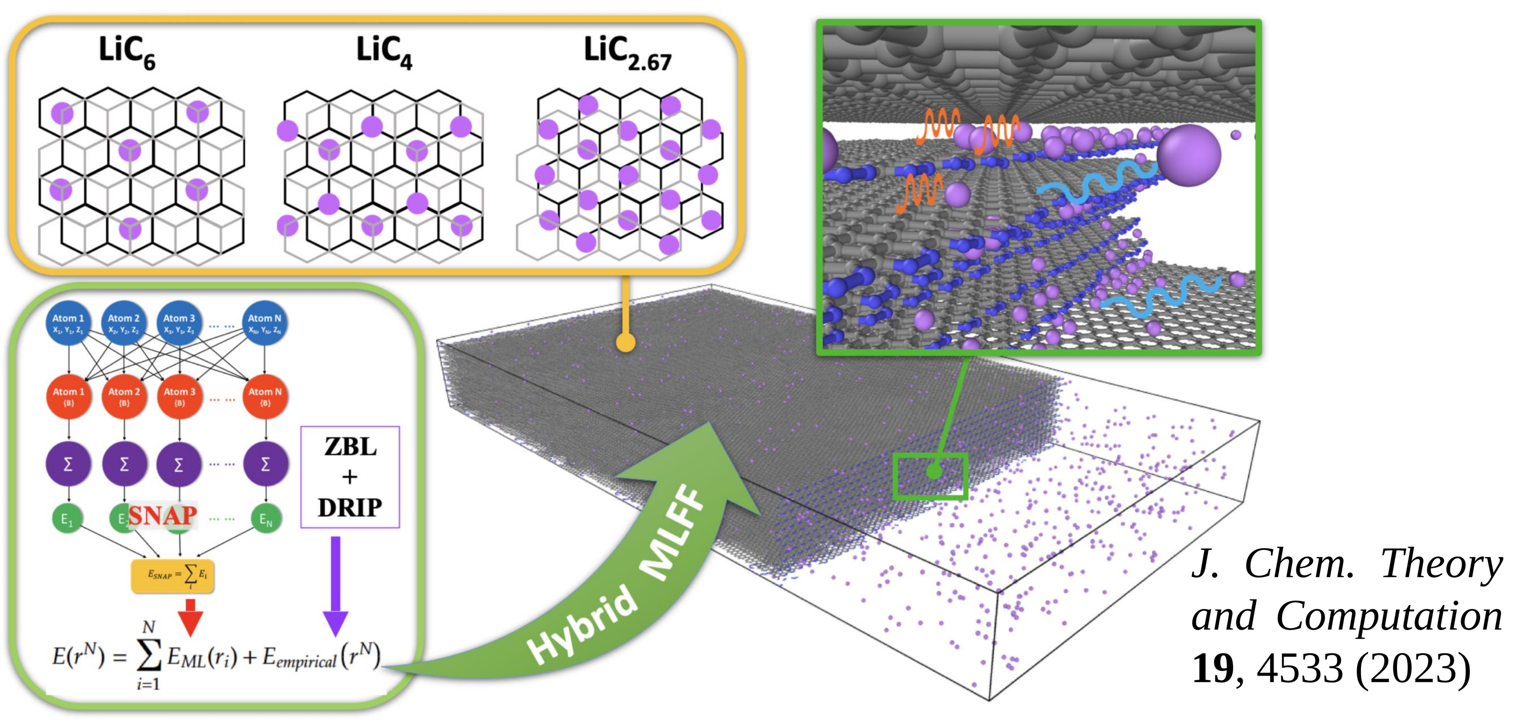


60 mAh Pouch Cell

A full cell (NCM622/CZTS) with 60 mAh is obtained in the pouch cell (57mm x 61 mm size).

Results and Discussion

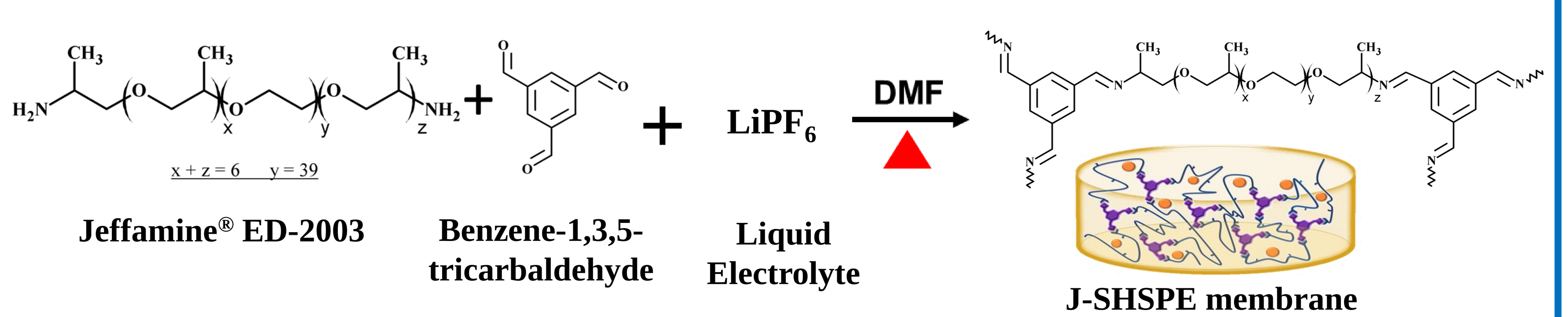
A hybrid machine learning energy model of lithium intercalation



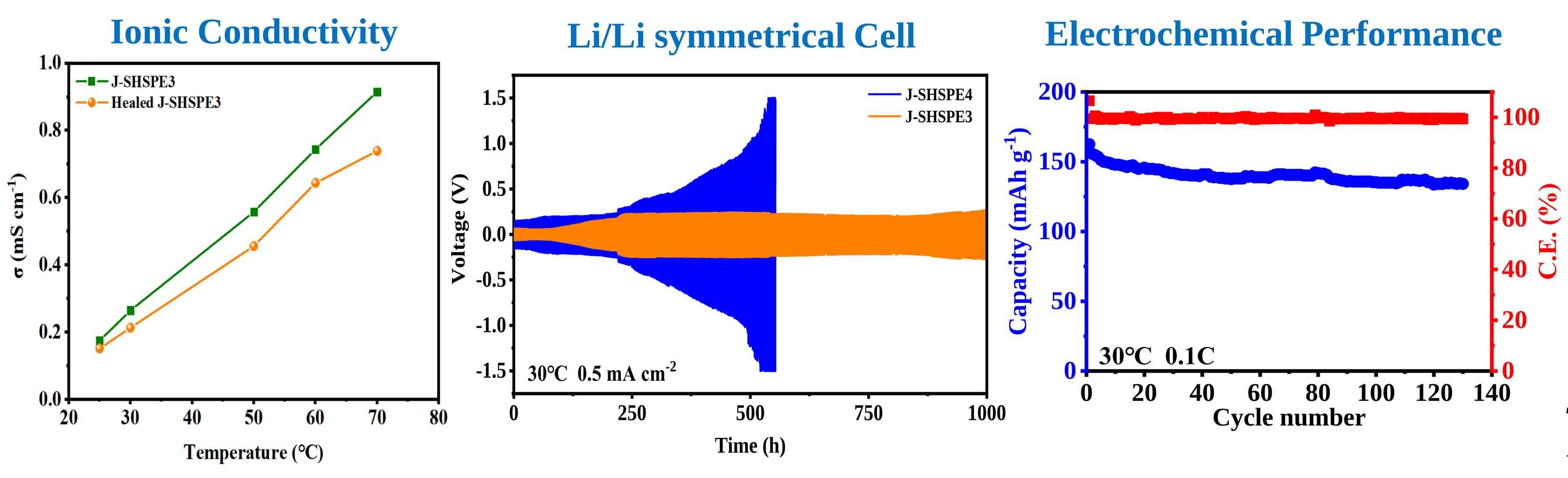
J. Chem. Theory and Computation **19**, 4533 (2023)

- A hybrid Machine learning energy model was developed to study lithium intercalation into graphite from plating to overlithiation
- The trained model can predict energy with high fidelity to DFT calculations. A new stable overlithiated phase LiC_4 is obtained from MD simulations

Jeffamine Based Self-Healable Solid Polymer Electrolyte



Schiff-base Reaction



At a low C-rate of 0.1C and at 30 °C, the LFP/J-SHSPE3/Li cell maintained ~134 mAh g^{-1} after 130 cycles.

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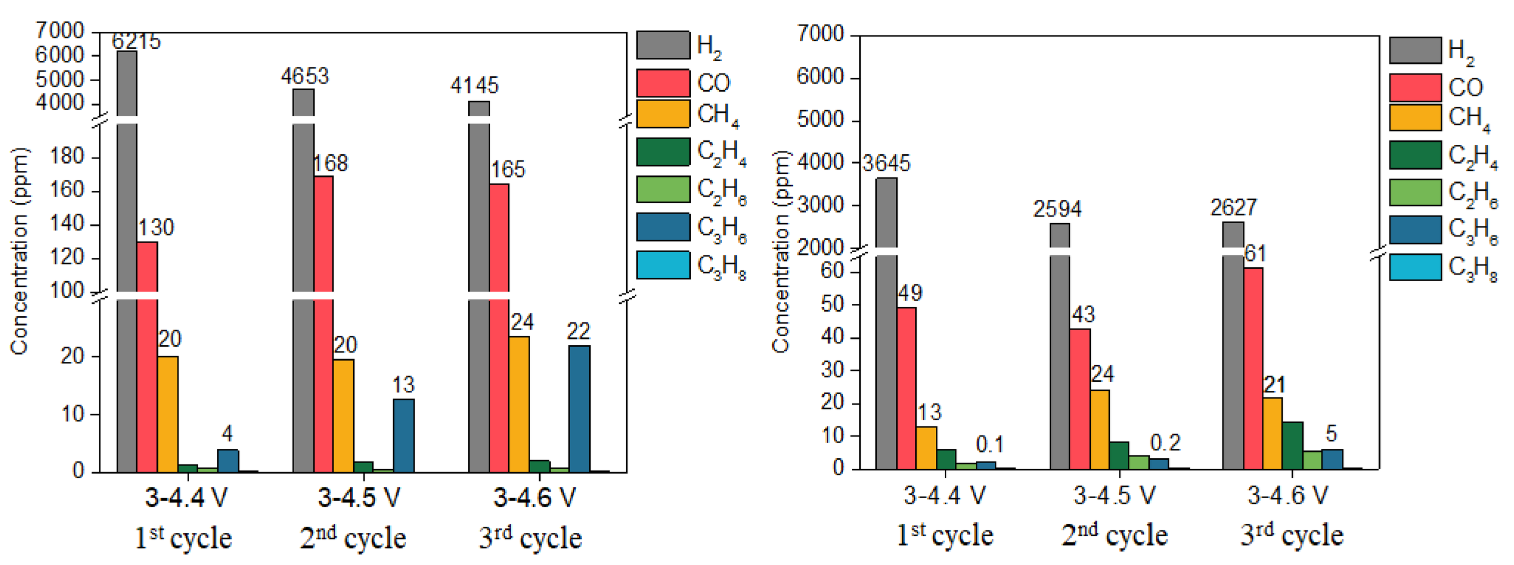
Results and Discussion

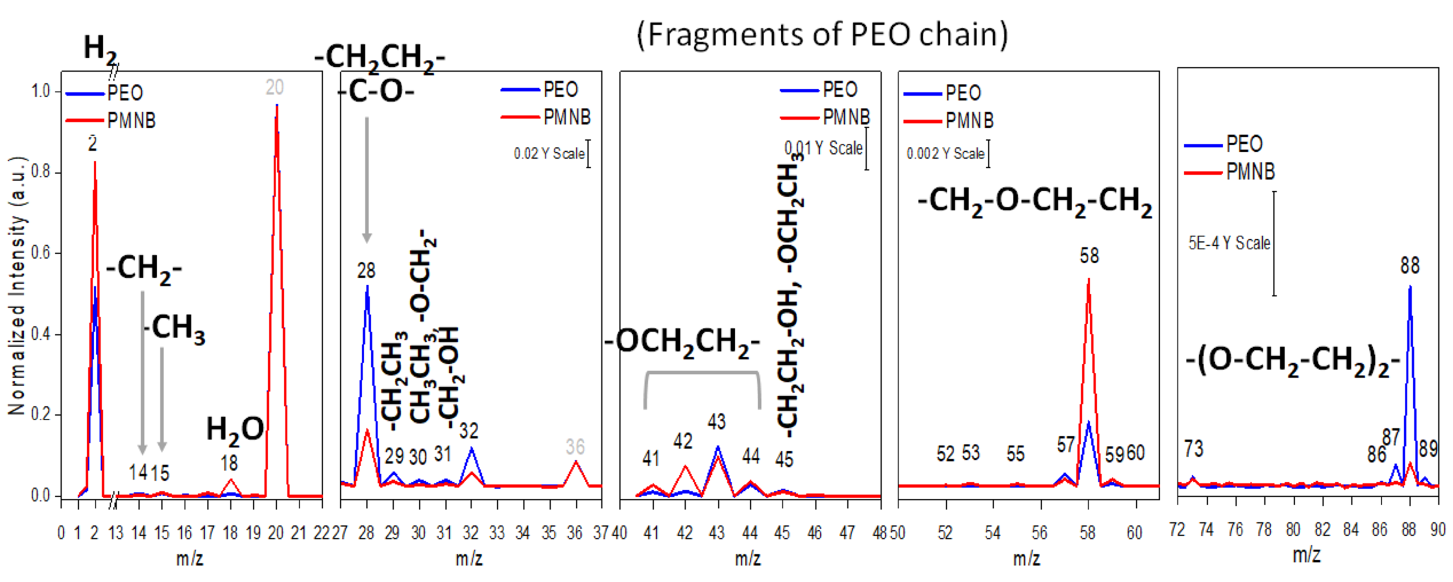
In situ gas chromatography and mass spectrometry measurements

Online GC measurements

Li/PEO/LiTFSI/NCM523 batteries　　Li/PMNBs/NCM523 batteries



Online mass spectrometry



Less gas evolution is obtained with PMNBs polymer electrolyte. PEO will be decomposed during cycling.

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