下世代鋰離子電池負極電極材料奈米結構技術

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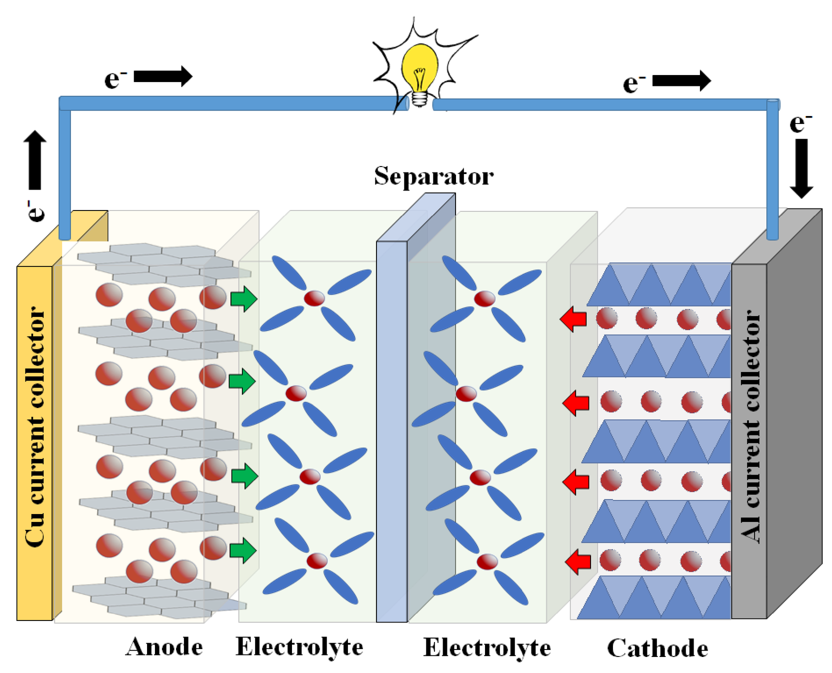
Abstract

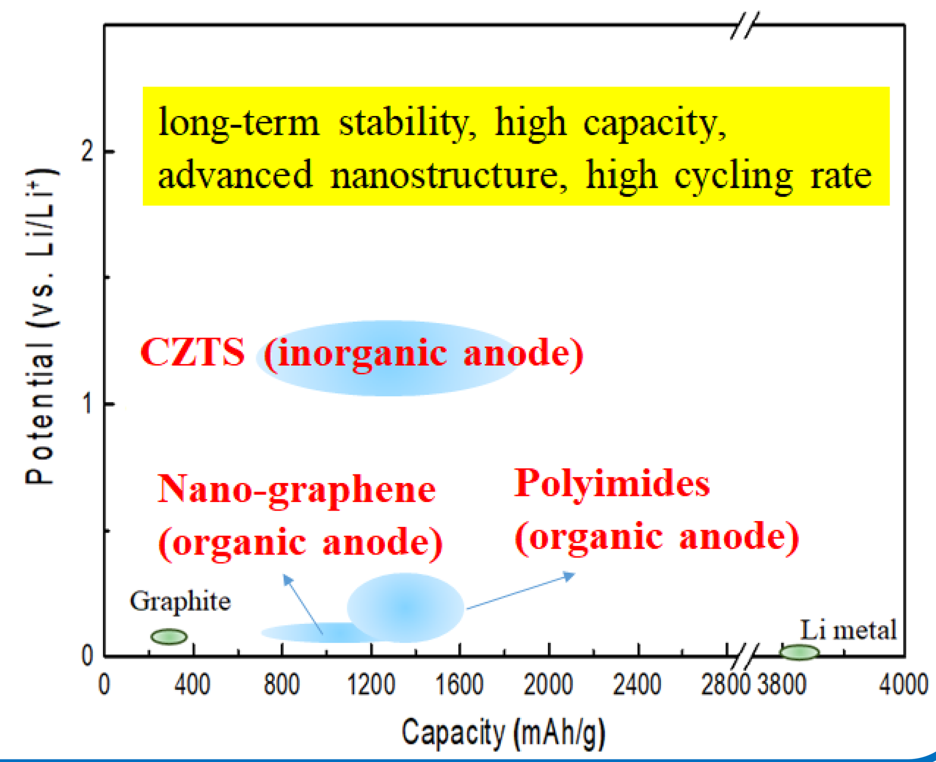
Global demand for rechargeable lithium-ion batteries has grown tremendously over the past two decades. However, lithium-ion batteries lack the higher capacity and longer life time required in electric vehicles and electricity infrastructure. In order to improve the energy density and extend the cycle 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

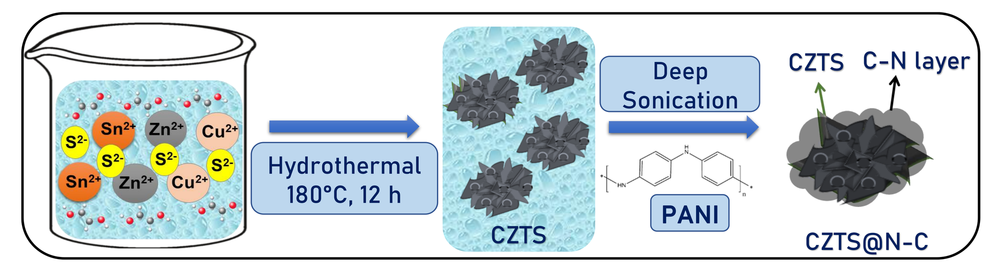


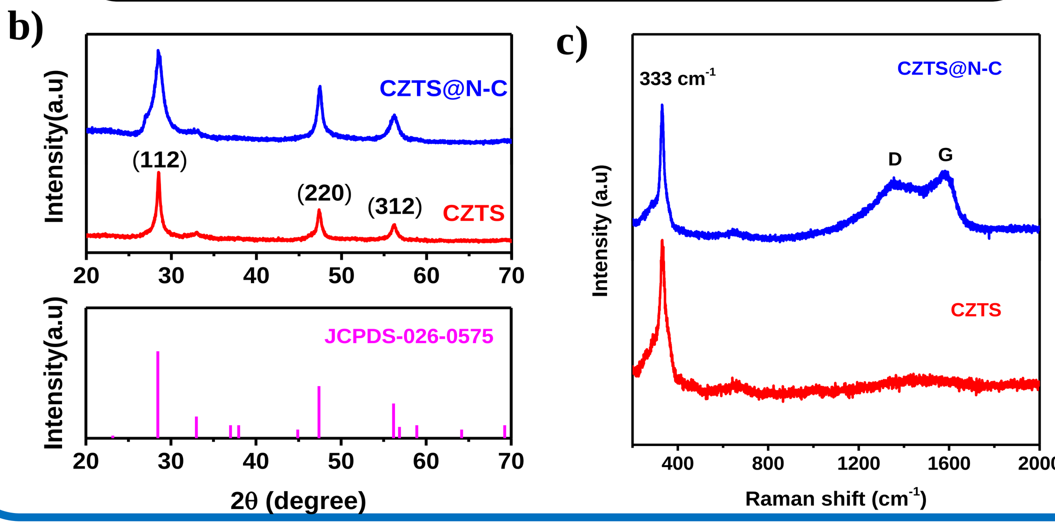
Anode materials



Results and Discussion

CZTS anode materials



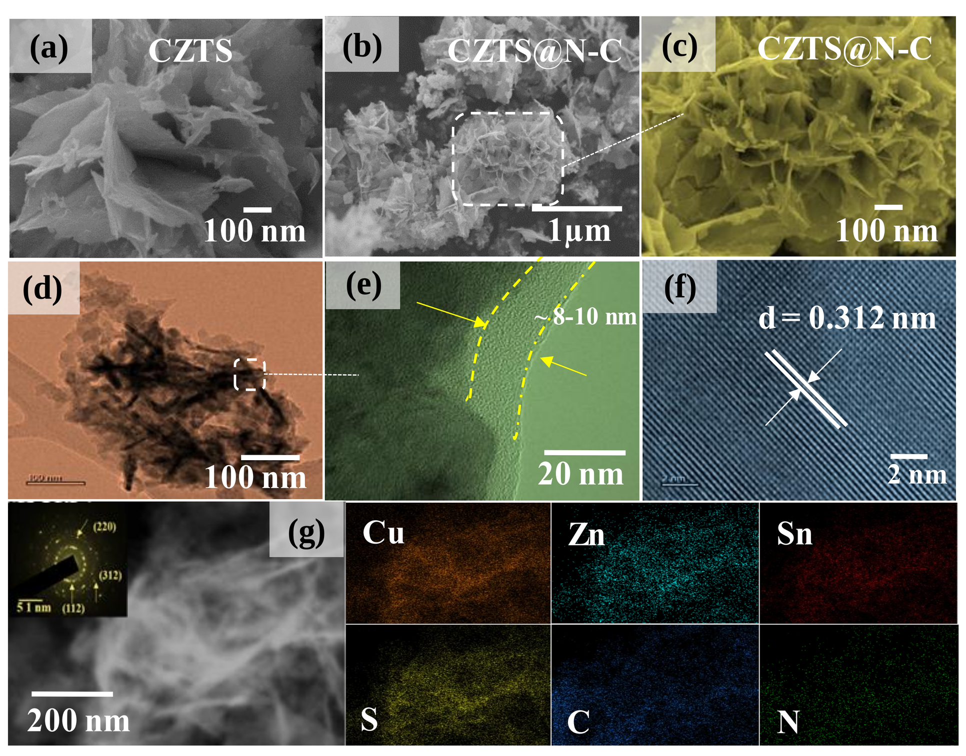


(a) The synthesis process of CZTS@N-C, (b) XRD patterns and (c) Raman spectra of CZTS and CZTS@N-C.

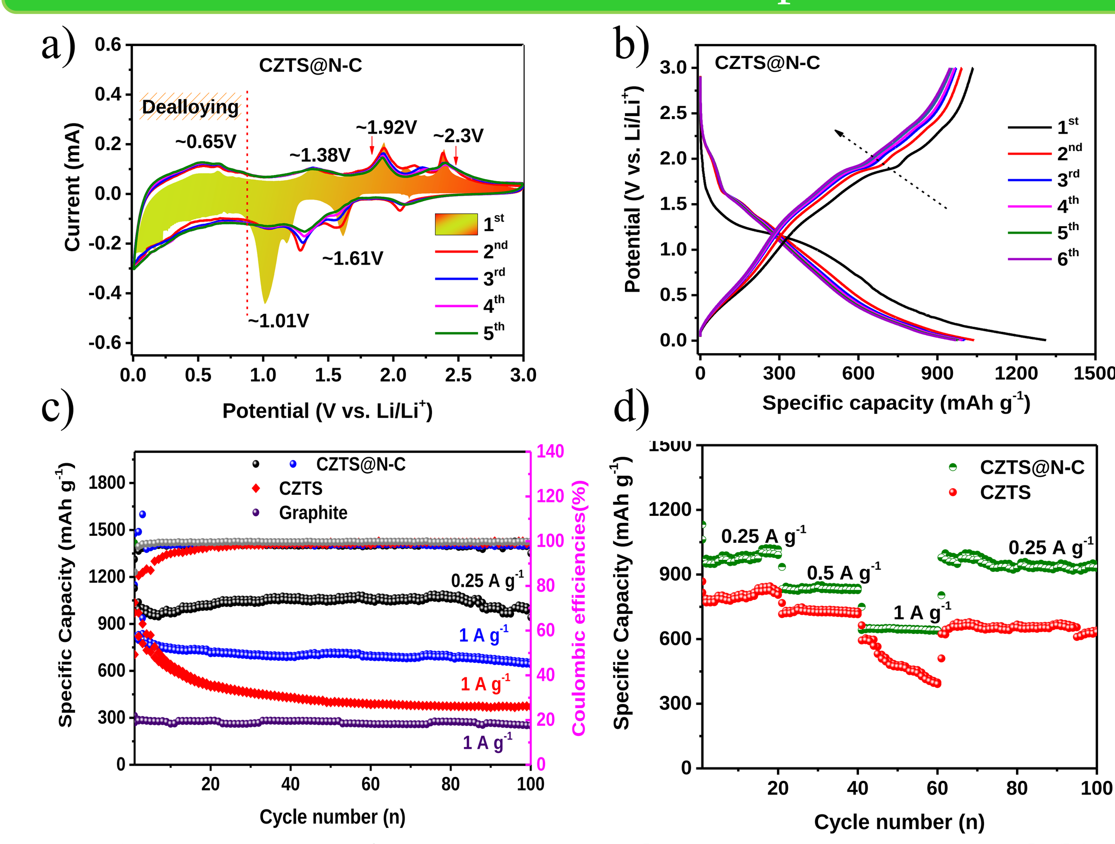
CZTS anode materials prepared by the hydrothermal method can be modified with different ligands and coatings.

Results and Discussion

CZTS anode materials and pouch cell demonstration



SEM image of (a) pristine CZTS and (b-c) CZTS@N-C composites (d) TEM image of CZTS@N-C, (e-f) The HRTEM images of CZTS@N-C composites. (g) The STEM-EDX elemental mapping of CZTS@N-C including dark-field images, Cu, Zn, Sn, S, C and N maps.

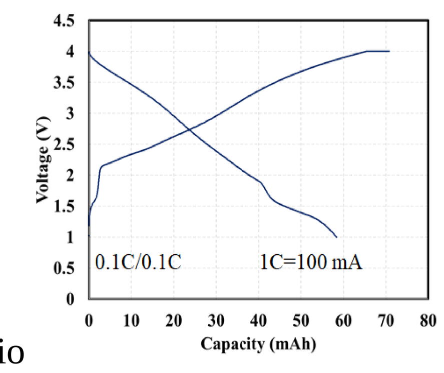


(a) CV curves of CZTS@N-C with 0.1 mV/s scan rate and (b) charge-discharge curves of CZTS@N-C at a rate of 1 A/g. (c-d) Electrochemical performance of CZTS, CZTS@N-C and graphite anode materials.

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 × 61 mm size).

Results and Discussion

Machine learning platform with quantuaccuracy

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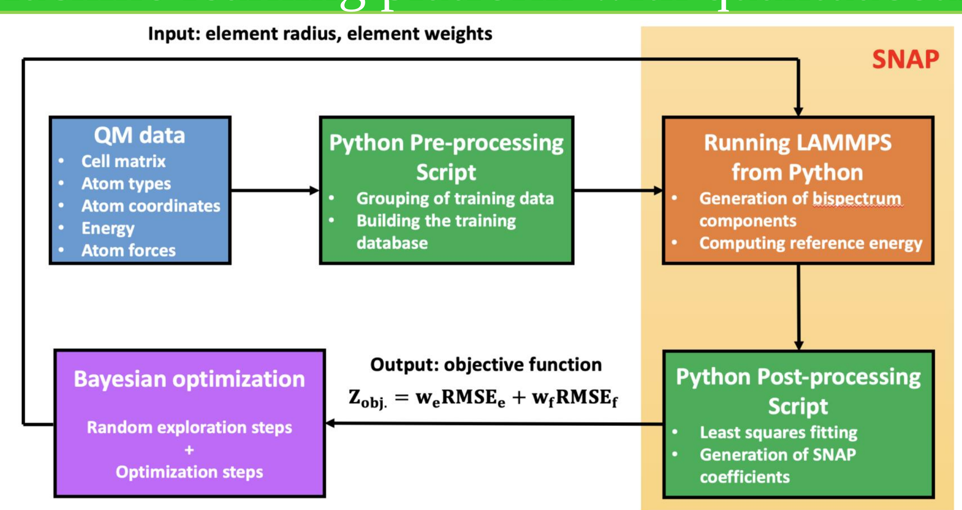
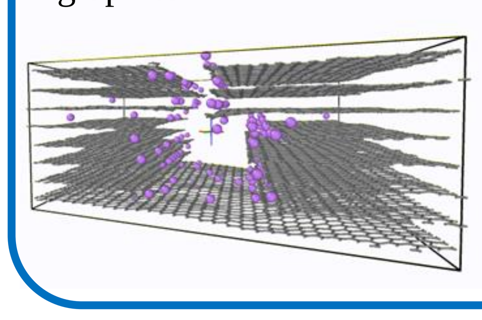
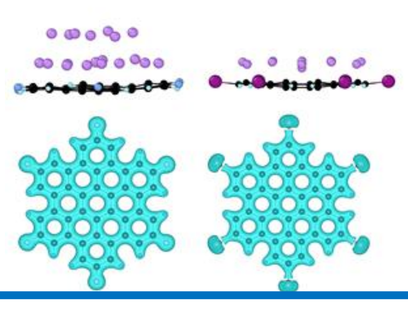


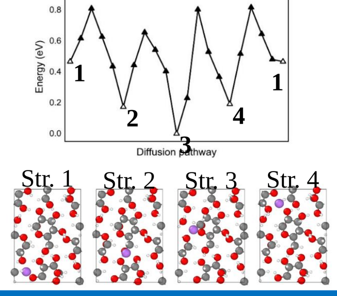
Intercalation vs. Plating of Li in graphite



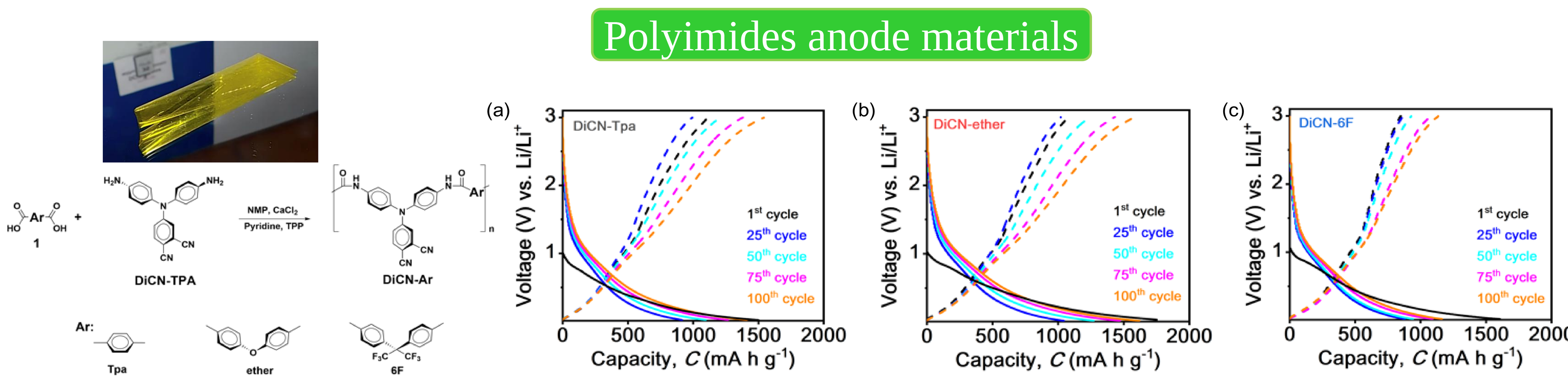
Li adsorption on F (left)/I(right) decorated nanographehe using DFT + AIMD calculations



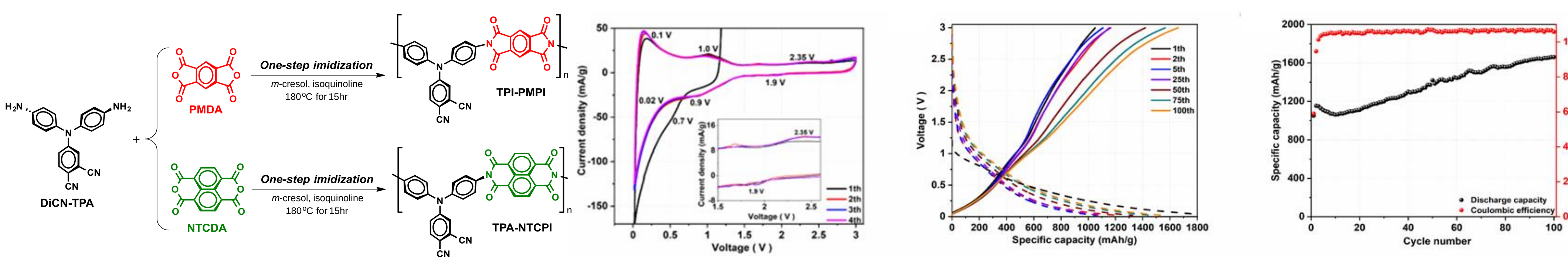
Li diffusion in Glucose artificial SEI layer using DFT + NEB calculations



Polyimides anode materials



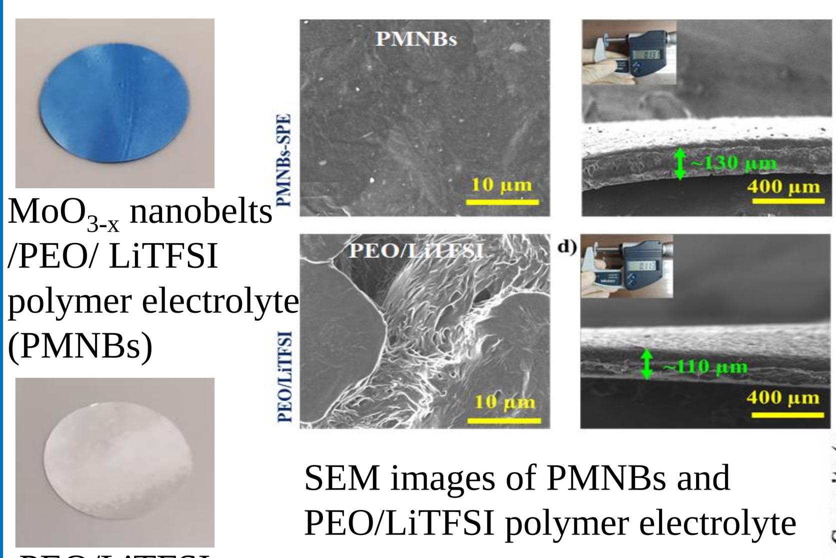
Synthetic route and charge-discharge curves of DiCN-PAs, DiCN-Tpa, DiCN-ether, and DiCN-6F.



Organic anode material shows a capacity of ~1600mAh/g after 100 cycles.

Results and Discussion

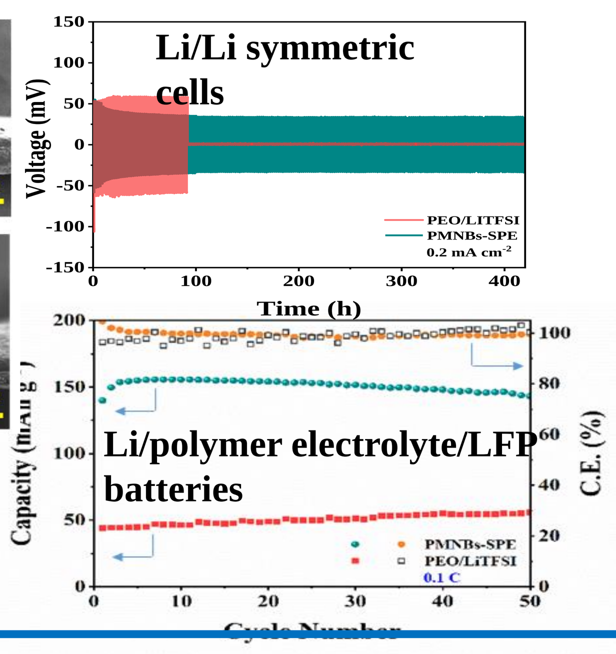
Solid-state polymer electrolyte and in situ characterizations



MoO_{3-x} nanobelts /PEO/ LiTFSI polymer electrolyte (PMNBs)

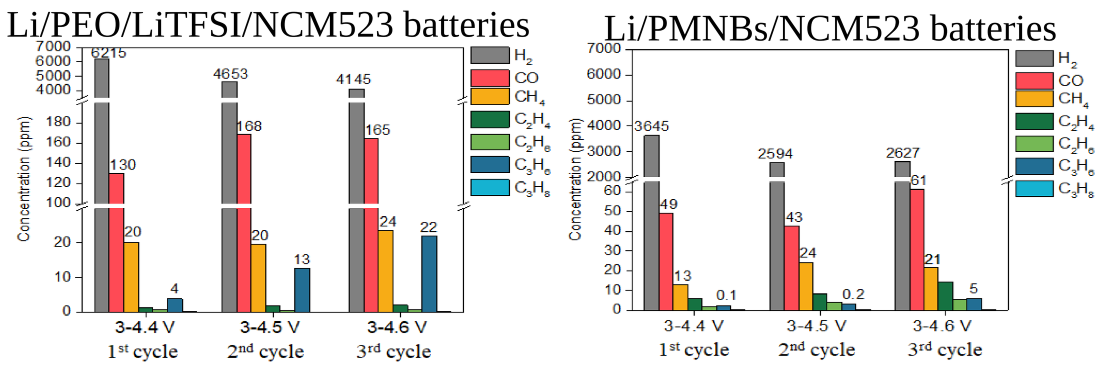
PEO/LiTFSI polymer electrolyte

SEM images of PMNBs and PEO/LiTFSI polymer electrolyte

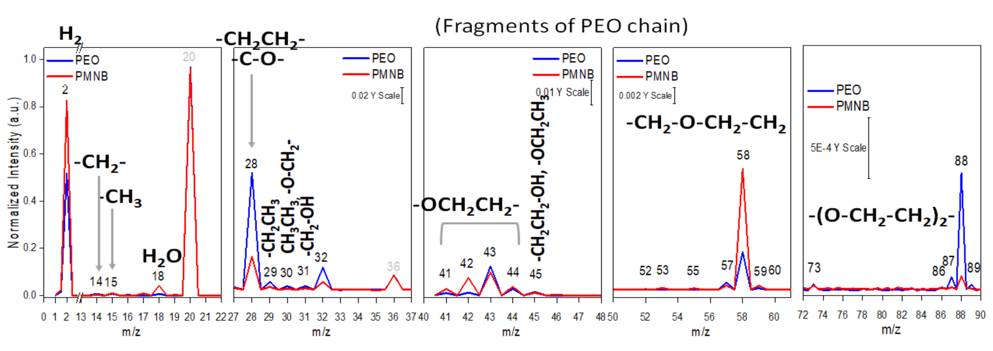


Online GC measurements

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.

Acknowledgements:

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