

Chemo-mechanical stable cathode interphase *via* interface in-situ catalytic-conversion integrated design for all solid-state batteries

*Xuanyi Zhou, Biao Zhang, Pengbo Lv, Lei Xi, Fangkun Li, Zengsheng Ma, Min Zhu, and Jun Liu**

X. Zhou, L. Xi, F. Li, M. Zhu, J. Liu

Guangdong Provincial Key Laboratory of Advanced Energy Storage Materials, School of Materials Science and Engineering, South China University of Technology, Guangzhou 510641, China.

E-mail: msjliu@scut.edu.cn (Jun Liu)

B. Zhang, P. Lv, Z. Ma

Key Laboratory of Low Dimensional Materials and Application Technology of Ministry of Education, School of Materials Science and Engineering, Xiangtan University, Xiangtan 411105, China.

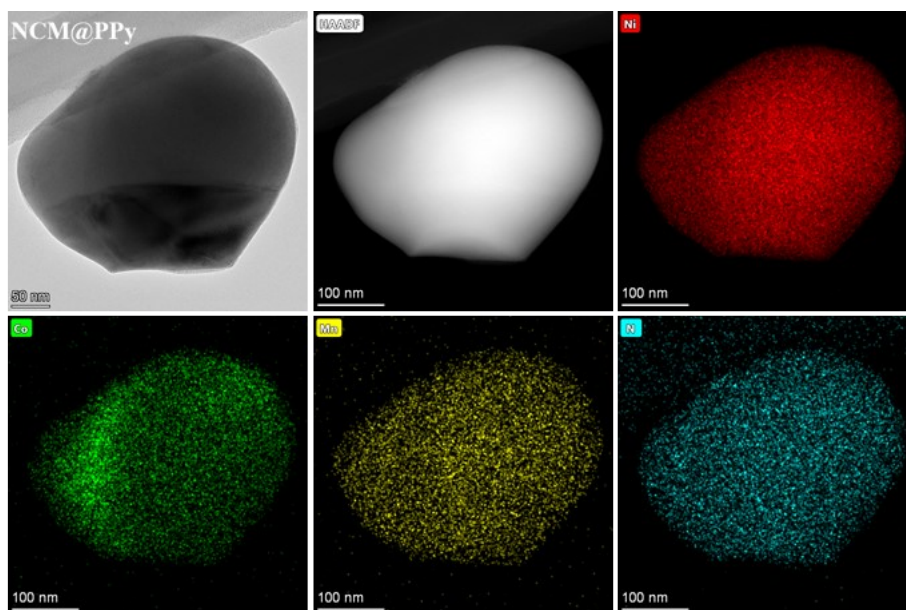


Figure S1. Morphology characterization. TEM and corresponding EDS mapping of NCM@PPy.

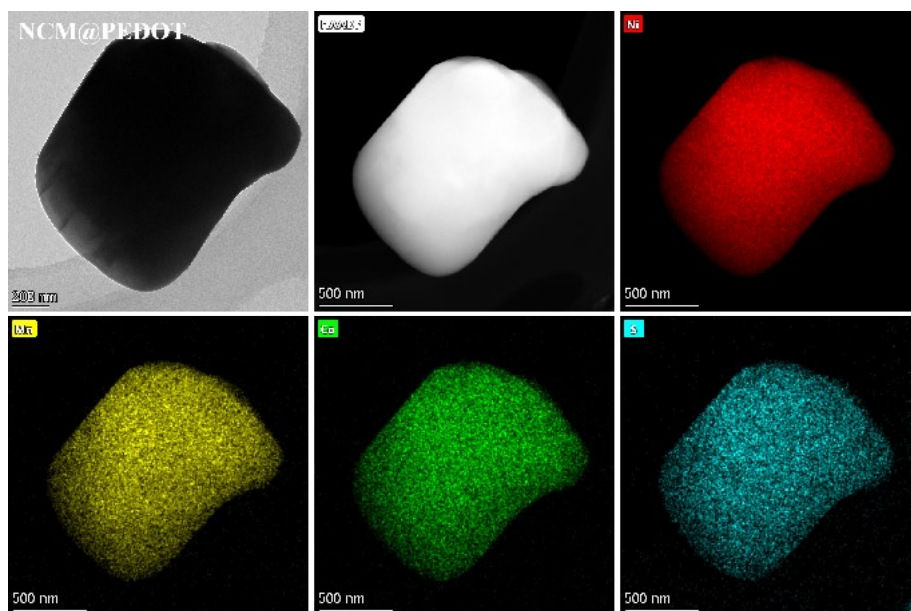


Figure S2. Morphology characterization. TEM and corresponding EDS mapping of NCM@PEDOT.

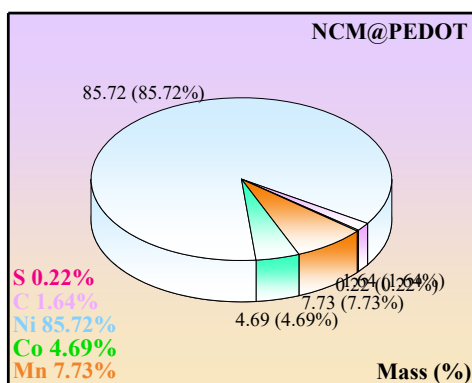


Figure S3. Elemental quantitative analysis. Element mass ratio diagram of NCM@PEDOT.

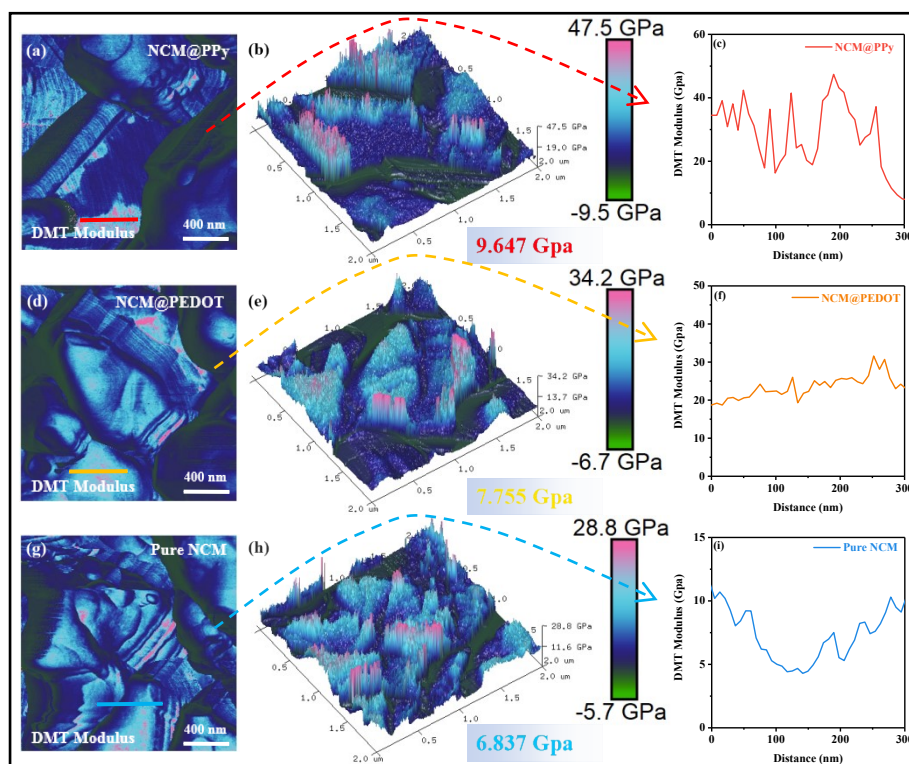


Figure S4. Young's modulus analysis of polymer coating. AFM Young's modulus mappings of (a) NCM@PPy, (d) NCM@PEDOT and (g) Pure NCM cathodes in the pristine state. 3D images of the modulus obtained in (b) NCM@PPy, (e) NCM@PEDOT and (H) Pure NCM cathodes and modulus curves of (c) NCM@PPy, (f) NCM@PEDOT and (i) Pure NCM. (The analysis area marked by the dashed line from Figure S1a, d, g)

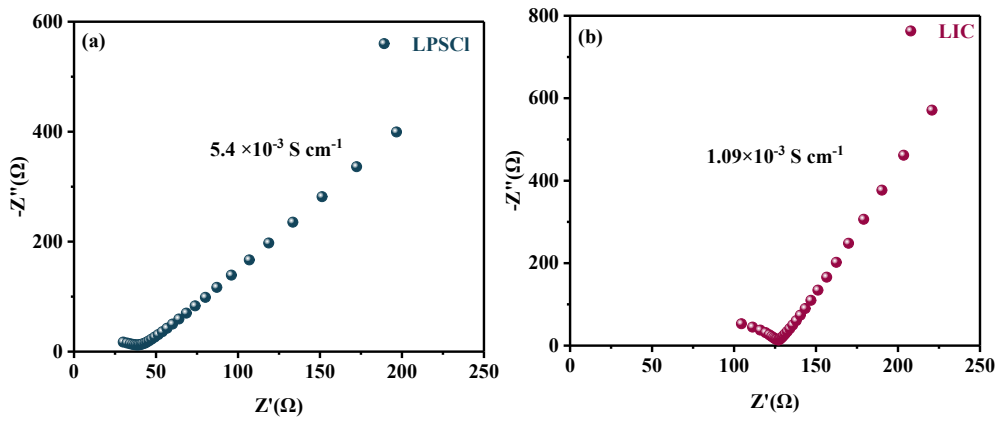


Figure S5. EIS measurement. (a) LPSCI. (b) LIC.

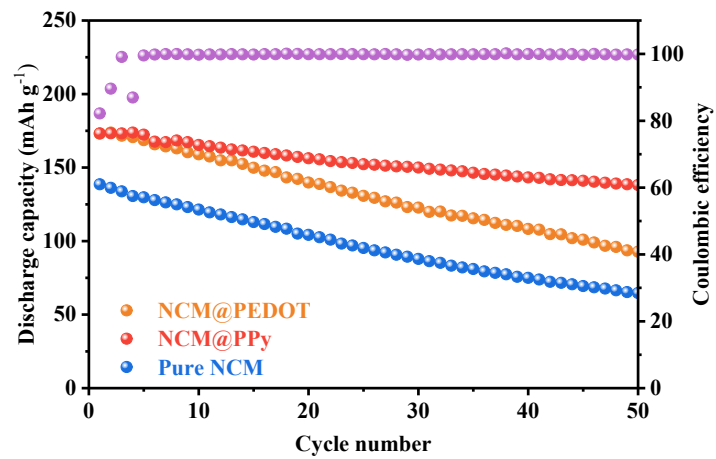


Figure S6. Battery performance. Cycling performance at 0.1C.

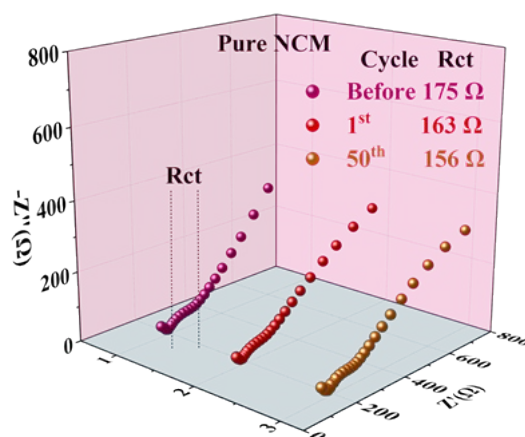


Figure S7. Battery impedance test. Electrochemical impedance spectroscopy of Pure NCM.

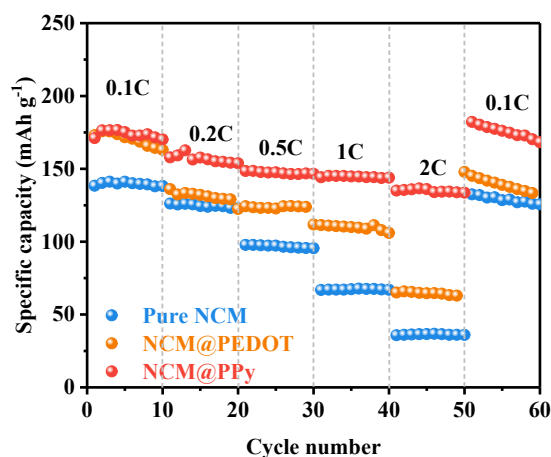


Figure S8. Cycling performance at different current density. Rate performance of NCM, NCM@PEDOT and NCM@PPy batteries.

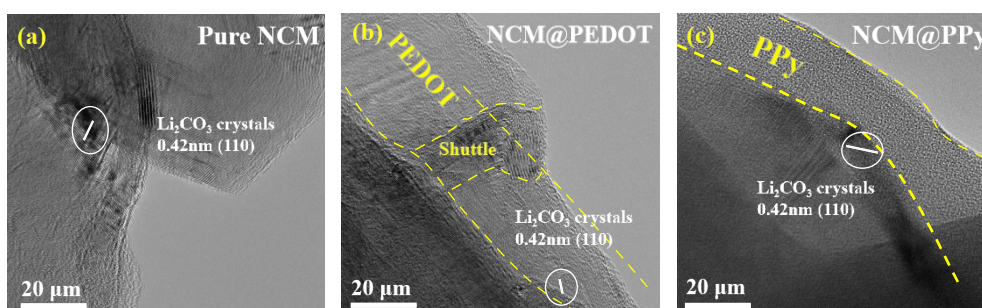


Figure S9. Interface product analysis after cycling. TEM of (a) Pure NCM, (b) NCM@PEDOT, (c) NCM@PPy after cycling.

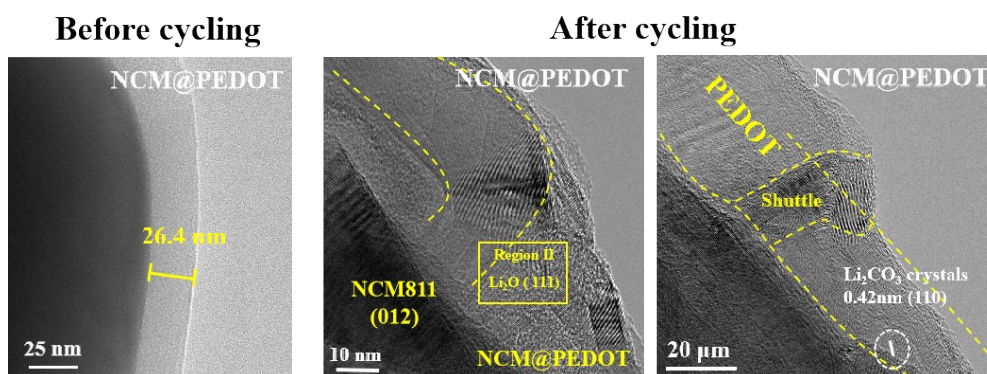


Figure S10. Interface product analysis before and after cycling. TEM of NCM@PEDOT before and after cycling.

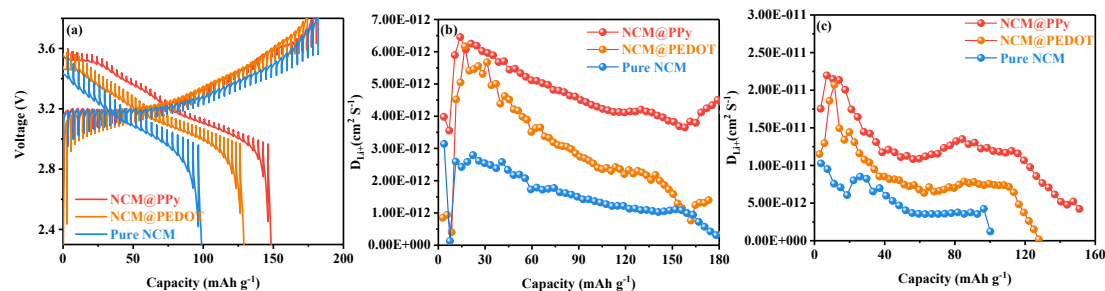


Figure S11. Li⁺ diffusion kinetics. (a) GITT test and D_{Li^+} at (b) charge and (c) discharge process of NCM@PPy, NCM@PEDOT, Pure NCM cathodes at the first cycle.

Table S1. Adsorption energy (E_{ads} , in eV) of Li⁺ on poly-pyrazole/thiophene systems.

Number of Li ⁺	pyrazole	thiophene
1Li ⁺	-2.30	-2.74
2Li ⁺	-2.22	-2.41

Table S2. Adsorption energy (E_{ads} , in eV) of Li₂O on poly-pyrazole/thiophene systems.

E_{des}/eV	pyrazole	thiophene
	5.08	0.77

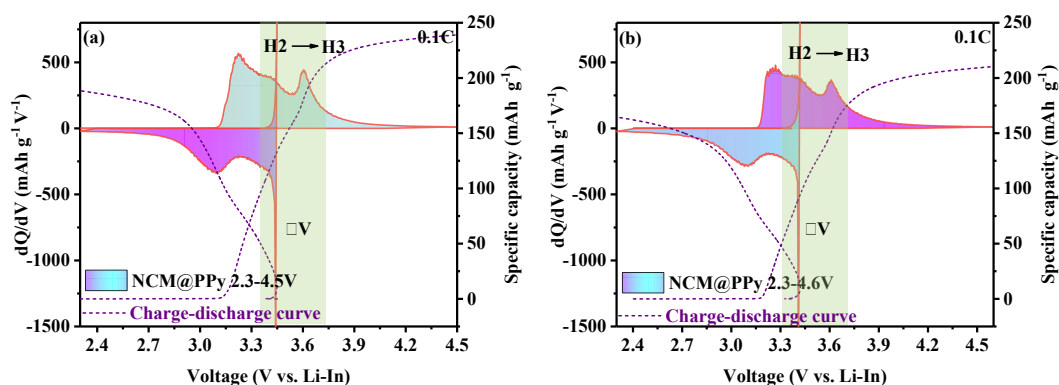


Figure S12. Initial charge-discharge potential curves and the dQ/dV profiles.

NCM@PPy battery performed at (a) 2.3-4.5V, (b) 2.3-4.6.

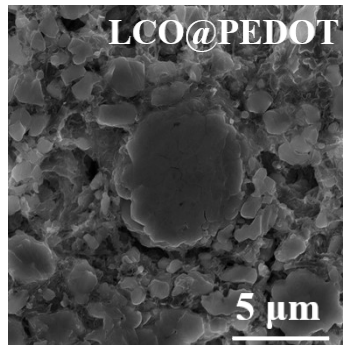


Figure S13. Microstructural evolution. FIB-SEM image of LCO@PEDOT cathode.

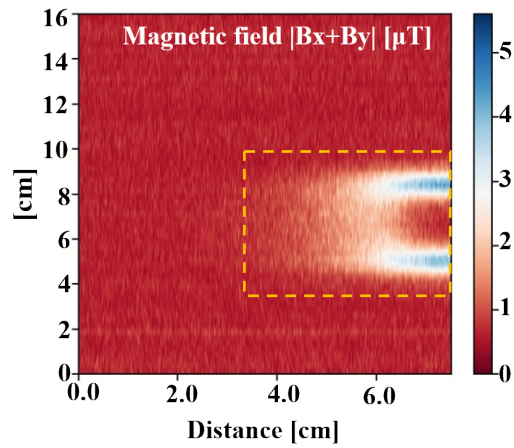


Figure S14. Magnetic Field Intensity (MFI) patterns. The distribution of the magnetic field mapping at $B_x + B_y$ of NCM@PPy pouch cell.