

Supporting Information

A functional electrolyte containing Propyl 4-methylbenzenesulfonate (PMBS) additive to improve the cycling performance of $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ / graphite full cell under the low-temperature of $-10\text{ }^{\circ}\text{C}$

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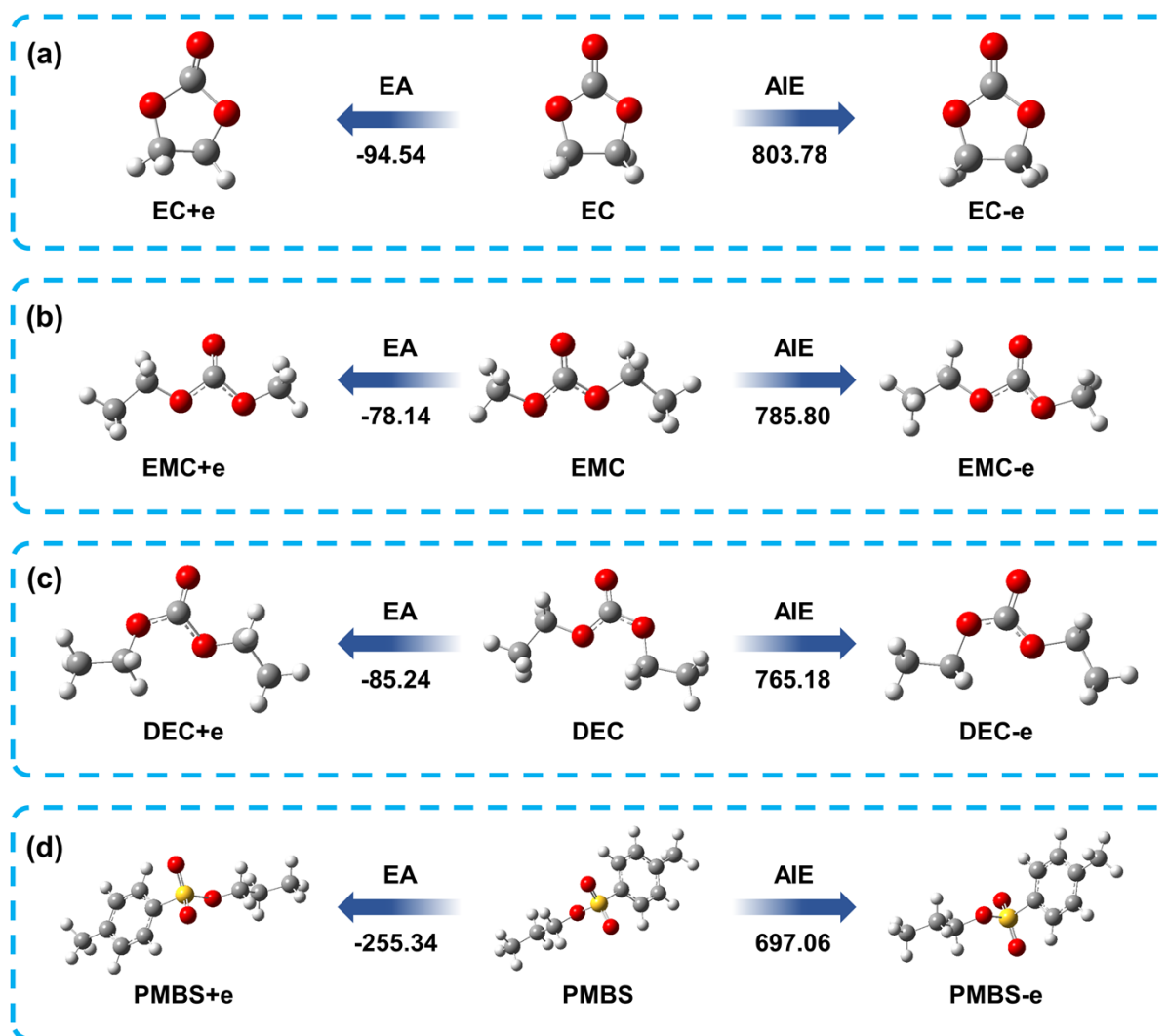


Fig. S1. Optimized structures and calculated electronic affinity energy (EA, kJ mol^{-1}) of (a) EC, (b) EMC, (c) DEC, (d) PMBS additive, as well as their adiabatic ionization energy (AIE, kJ mol^{-1}).

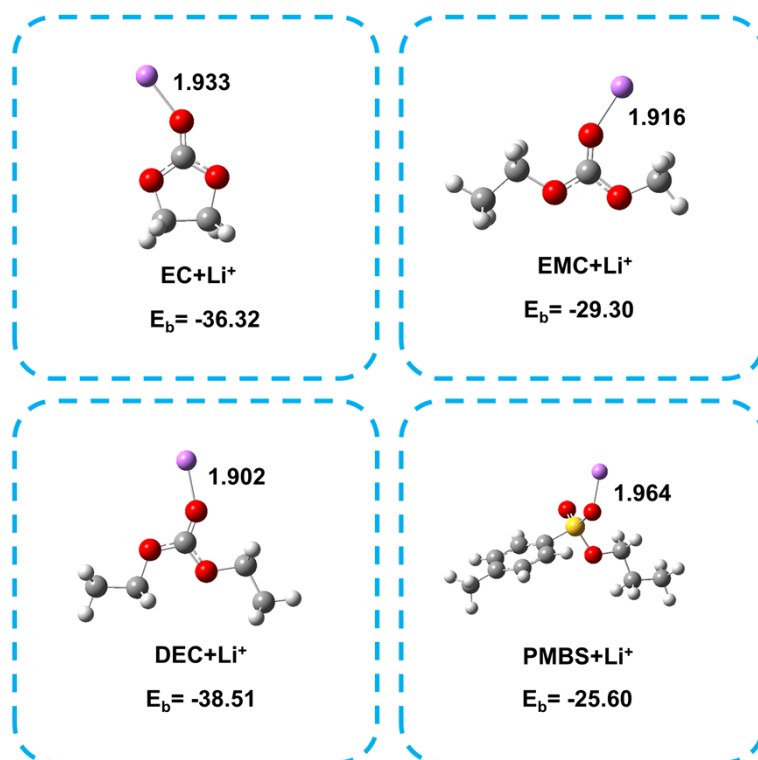


Fig. S2. Optimized structures and calculated binding energy (E_b , kJ mol⁻¹) between Li⁺ with electrolyte solvent or PMBS additive.

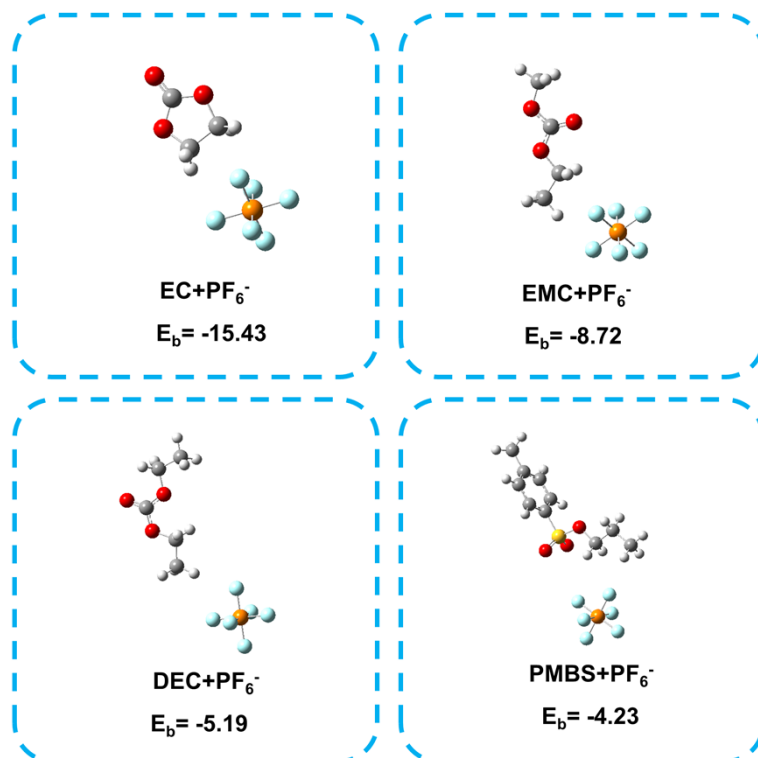


Fig. S3. Optimized structures and calculated binding energy (E_b , kJ mol^{-1}) between PF_6^- with electrolyte solvent or PMBS additive.

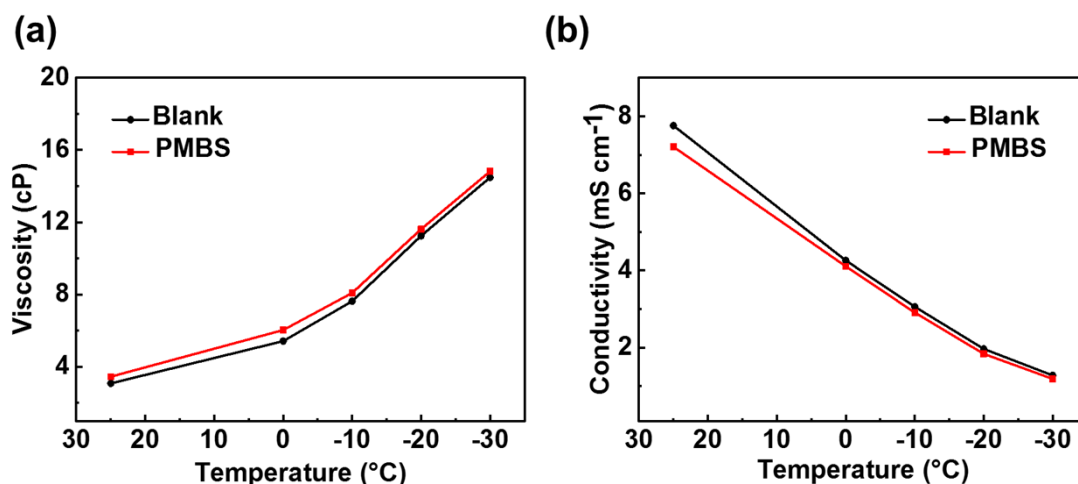


Fig. S4 (a) Viscosity and (b) conductivity of the electrolyte without and with 2% PMBS at different temperature.

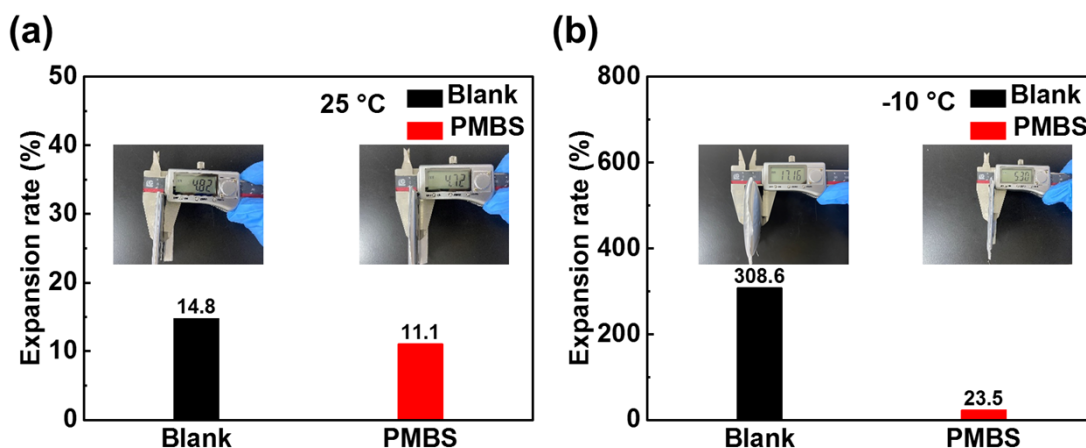


Fig. S5 The expansion rate and the corresponding photographs of the NCM811/graphite pouch full cells after (a) 1200 cycles at 25 $^{\circ}\text{C}$, (b) 100 cycles at -10 $^{\circ}\text{C}$

The thickness of the pouch cells before (T_0) and after (T_1) the cycle were tested. The expansion rate (T_r) was calculate according the formula as follow: $T_r = (T_1 - T_0) / T_0$.

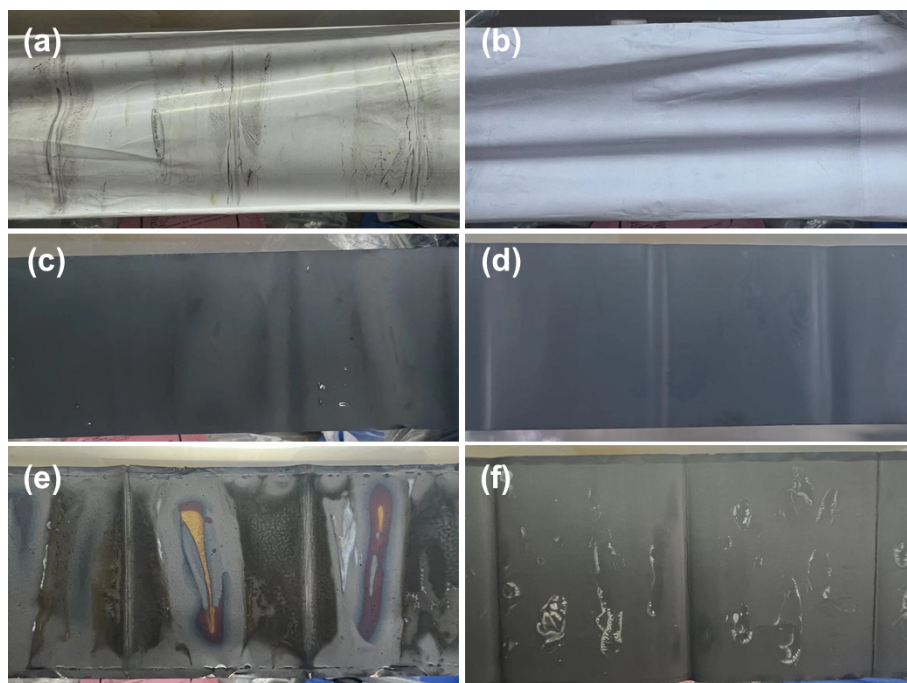


Fig. S6. Photographs of the separators, NCM811 cathode and graphite anode from the cells after 100 cycles at -10 °C. (a, c, e) Blank electrolyte, (b, d, f) PMBS-containing electrolyte.

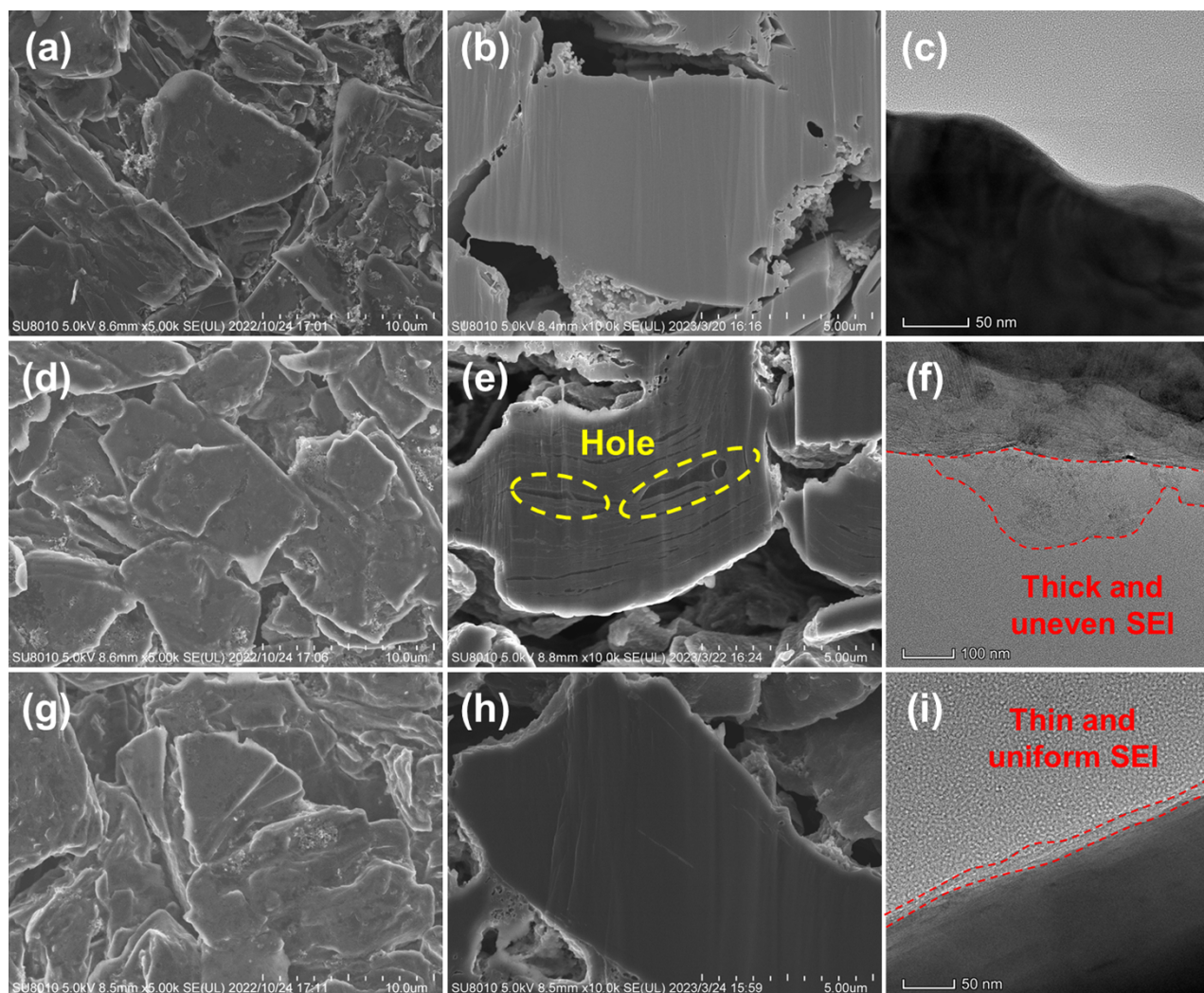


Fig. S7. The SEM images of the surface morphology and cross-section of graphite anode as well as the corresponding TEM images. (a-c) Fresh graphite anode. (d-f) The graphite anode after 100 cycles at -10 °C from the cell with blank electrolyte. (g-i) The graphite anode after 100 cycles at -10 °C from the cell with 2% PMBS-containing electrolyte.

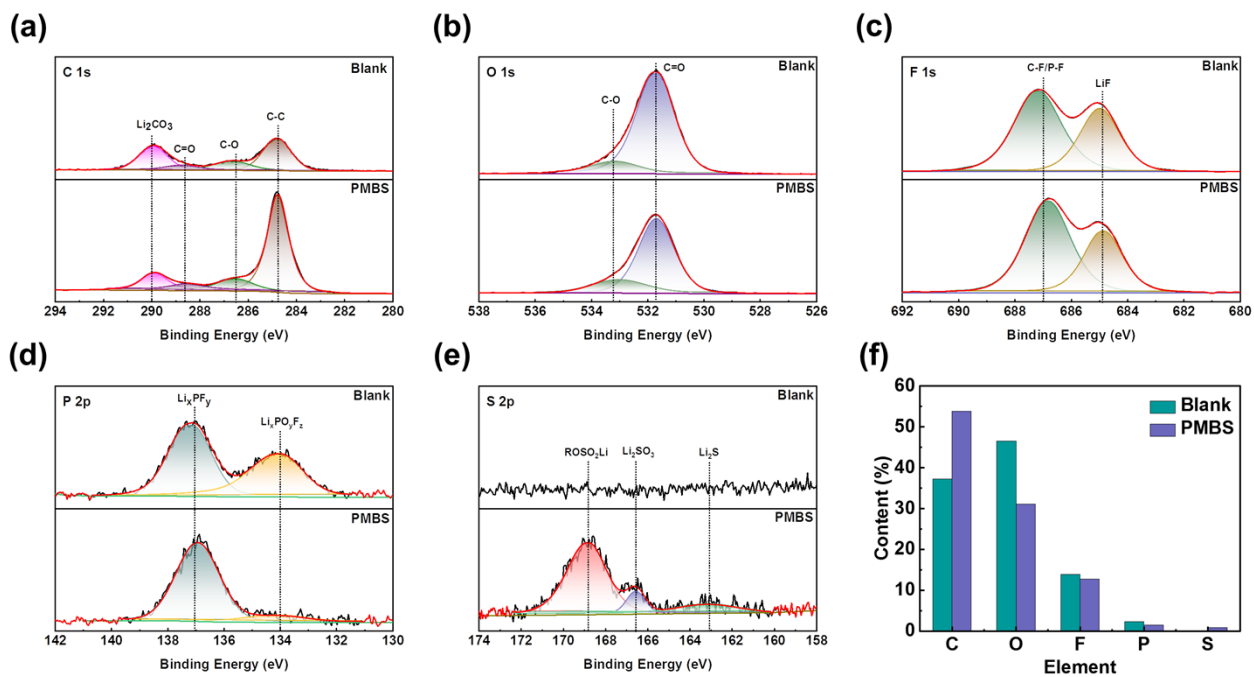


Fig. S8. XPS spectra of (a) C 1s, (b) O 1s, (c) F 1s, (d) P 2p, and (e) S 2p for the anodes obtained from the cells with different electrolyte after cycling at $-10\text{ }^{\circ}\text{C}$. (f) The contents of different elements on the cathode surface obtained by XPS analysis.

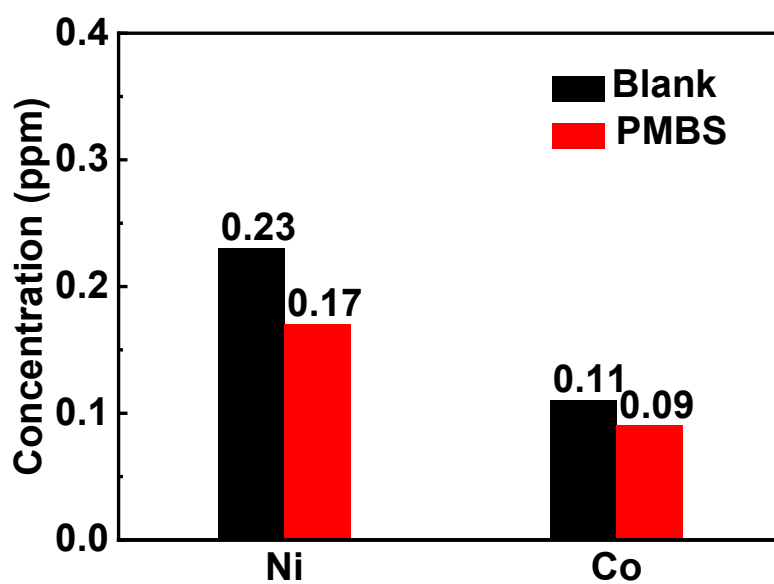


Fig. S9. The amount of transition metal deposited on the graphite anode of the cell after cycling in different electrolytes.

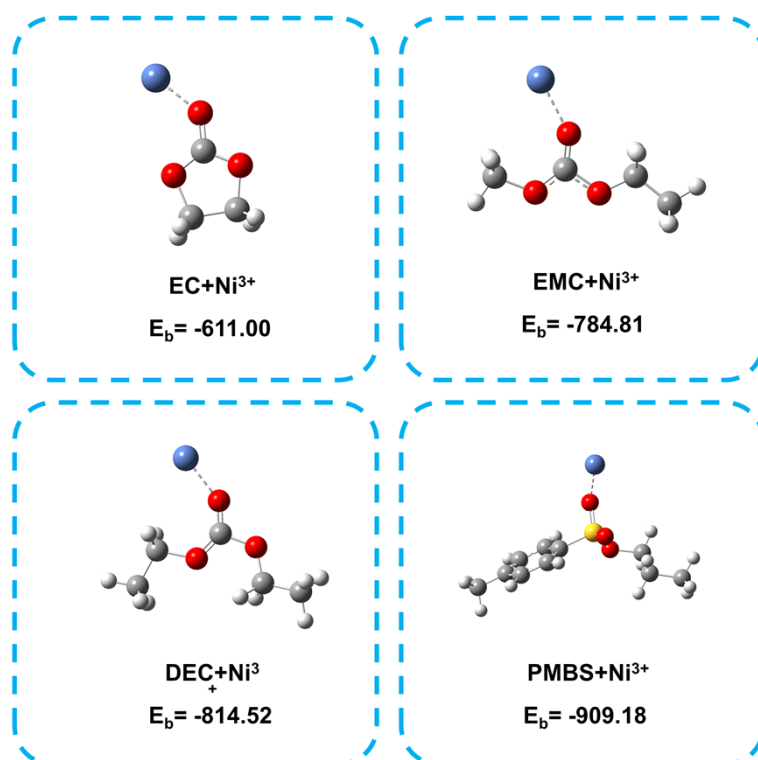


Fig. S10. Optimized structures and calculated binding energy (E_b , kJ mol⁻¹) between Ni³⁺ with

electrolyte solvent or PMBS additive.

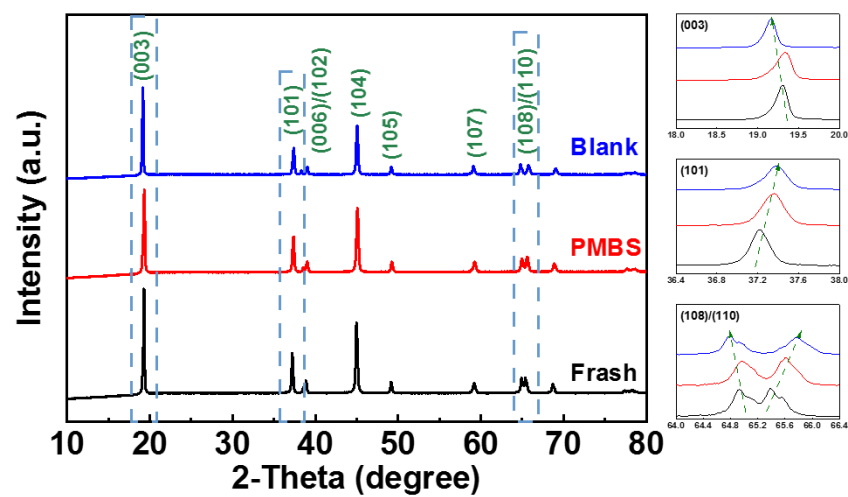


Fig. S11 The XRD patterns of fresh and cycled NCM811 cathode obtained from the NCM811/graphite pouch full cells with different electrolyte after 100 cycles at -10 °C.