

Supporting Information

Construction of a Stable $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ (NCM811) Cathode Interface by a Multifunctional Organosilicon Electrolyte Additive

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Table S1. HOMO and LUMO energies of EC, EMC, BSA and the chemical reaction products.

eV	EC	EMC	BSA	TMSO	TMSN	NAO	TMSF
HOMO	-8.4676	-8.0927	-6.4994	-7.4186	-6.674	-7.7686	-8.4894
LUMO	-0.6035	-0.4234	-0.5516	-0.5219	-0.6193	-0.6460	-0.4547

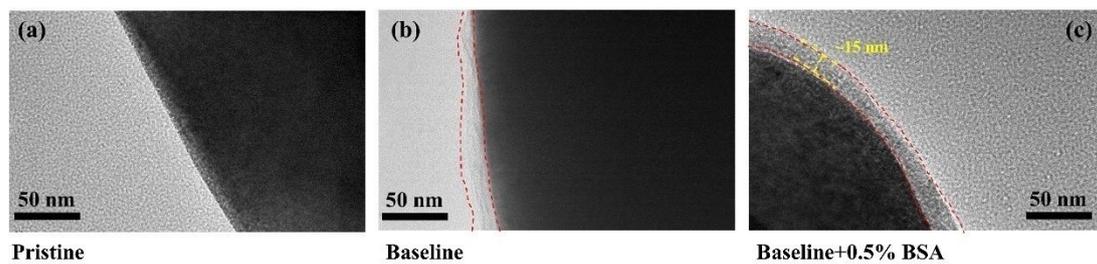


Figure S1. TEM images of pristine NCM811 electrode (a) and the NCM811 electrodes after formation process cycles at 0.1 C rate with Baseline (b) and Baseline+0.5% BSA (c) electrolytes.

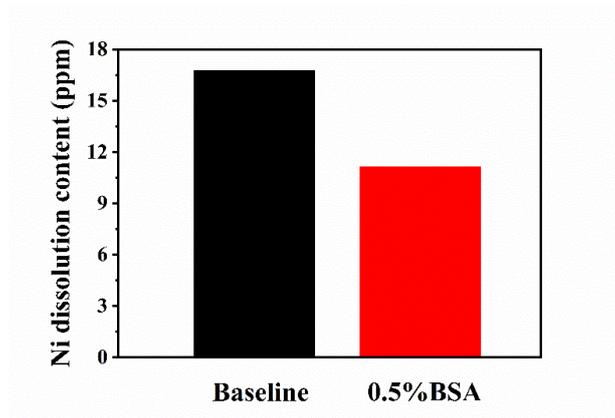


Figure S2. The content of Ni deposited on the cycled lithium anode with and without BSA additive.

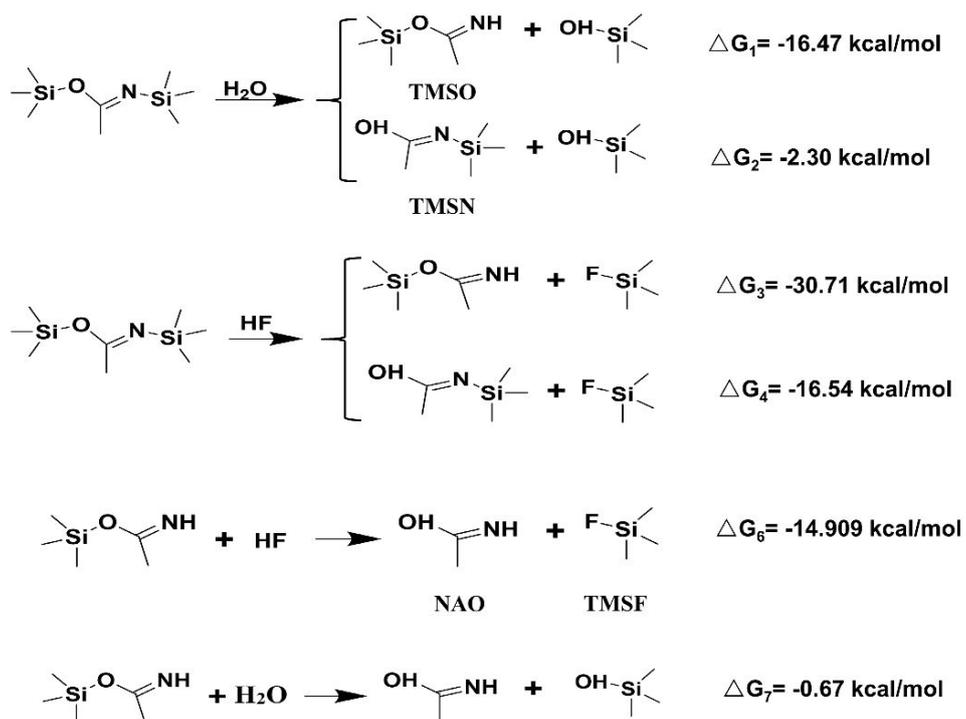


Fig S3. ΔG in kcal/mol for reactions of BSA with H_2O and HF .

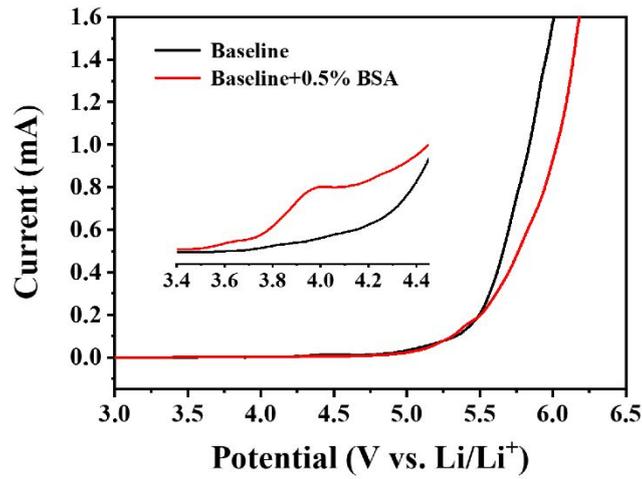


Figure S4. LSV curves of Baseline and Baseline + 0.5% BSA electrolytes were tested between open-circuit-potential and 6.5 V.

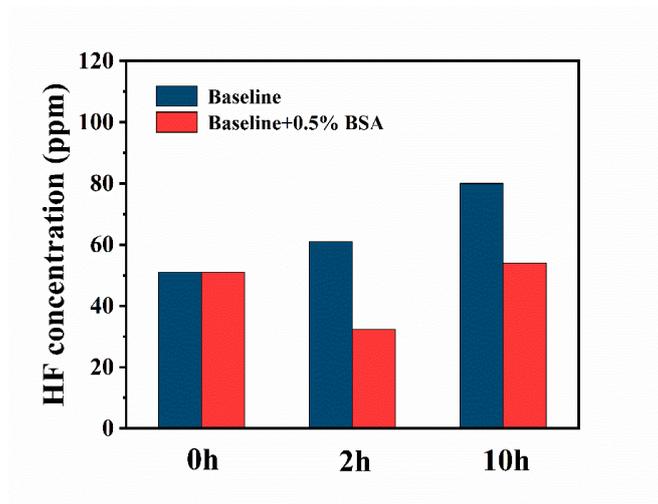


Figure S5. HF concentration generated in the baseline and 0.5% BSA electrolytes at different storage times.