

Supporting Information

for

Na_{0.5}Bi_{0.5}TiO₃ Perovskite Anode for Lithium Ion Battery

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Table S1. Crystallographic parameters derived from the Rietveld refinement of lab XRD data (Cu K α) of Na_{0.5}Bi_{0.5}TiO₃ at 25 °C.

Formula	Na _{0.5} Bi _{0.5} TiO ₃					
Crystal system	<i>Trigonal</i>					
Space group	<i>R3c</i> (#161)					
Unit cell parameter (Å)	$a = b = 5.4844, c = 13.50305$					
Unit cell volume (Å ³)	$V = 351.744$					
Theoretical density (g/cm ³)	6.001					
Refinement factors	$R_{\text{Bragg}} = 2.34\%, \text{Global } \chi^2 = 24$					
Atom	Wyckoff Position	x/a	y/b	z/c	Occupancy	$B_{\text{iso}}/\text{Å}^2$
Na	6a	0	0	0.3	0.5	1.73(63)
Bi	6a	0	0	0.3	0.5	1.73(63)
Ti	6a	0	0	0	1	-0.47(12)
O	18b	0.1286(63)	0.2921(60)	0.1124	1	1

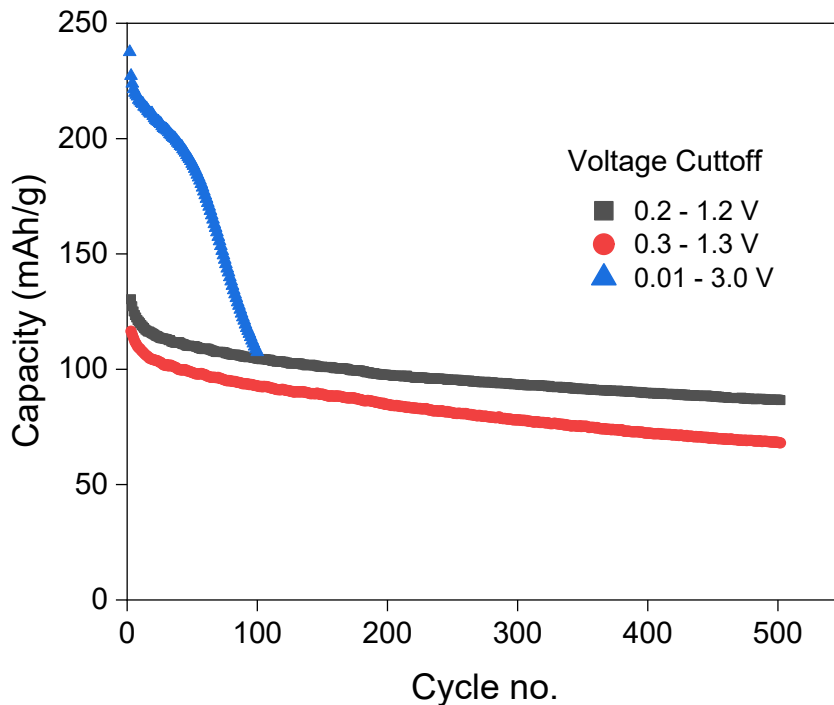


Figure S1. Cycling performance of NBT perovskite anode in different voltage windows: (0.01-3.0 V) -red, (0.2-1.2 V) - green, and (0.3-1.3 V) – blue.

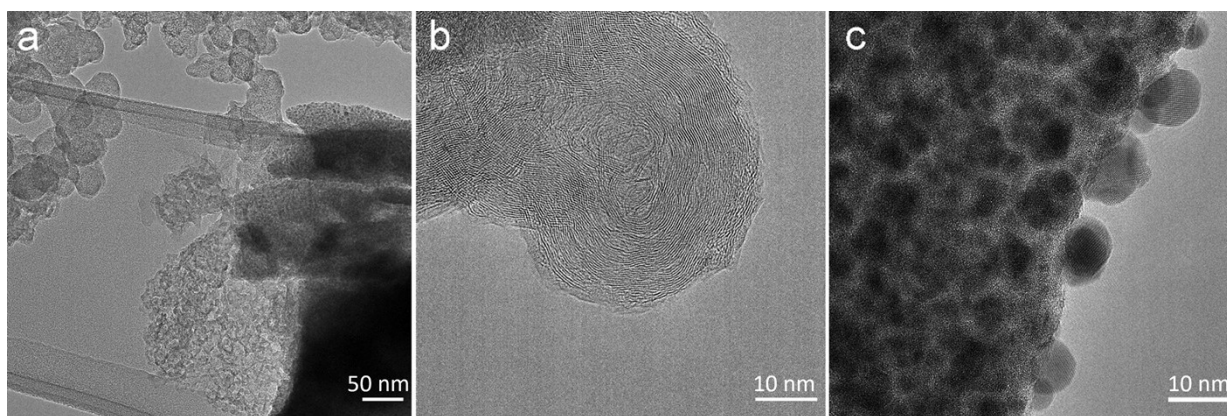


Figure S2. TEM images of the 1C sample: (a) mixture of conductive carbon, parent $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ and Li_2O , (b) magnified image of conductive carbon, and (c) magnified image of the surface of pristine $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$.

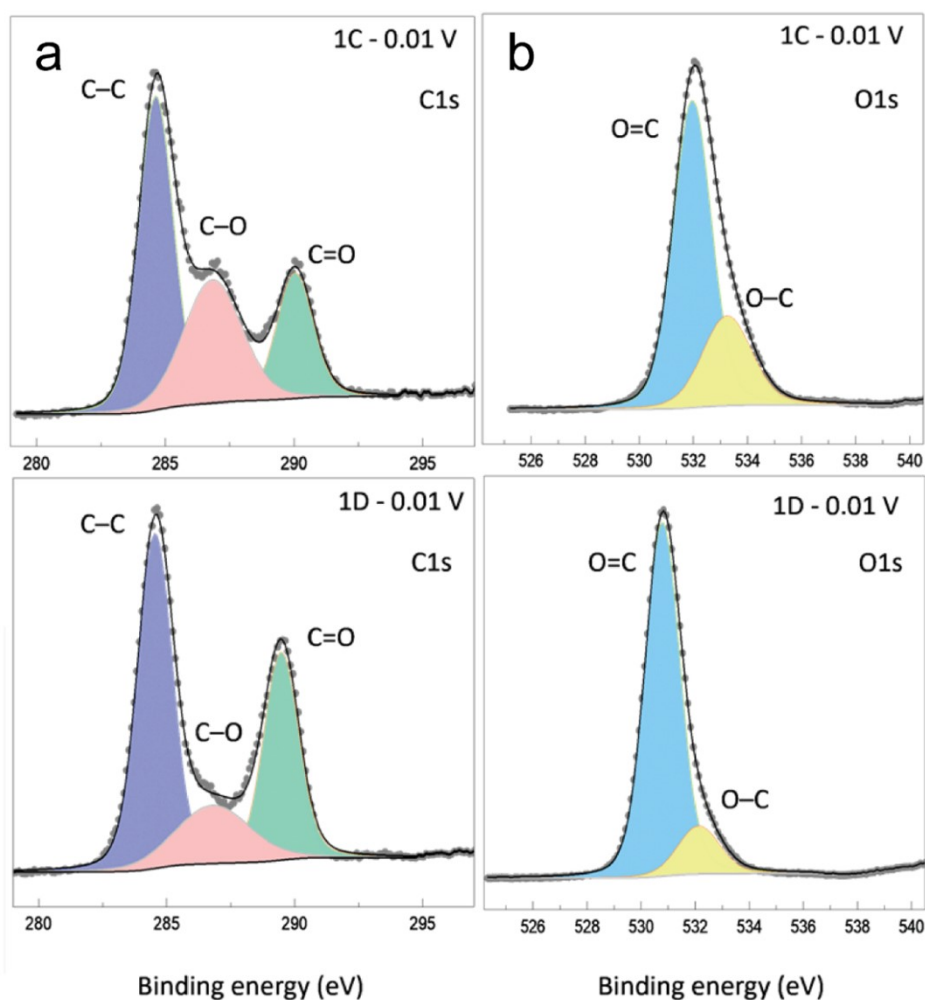


Figure S3. Ex-situ XPS study showing (a) C 1s spectra after full charge (top) and full discharge (bottom); and (b) O 1s spectra after full charge (top) and full discharge (bottom).