Electronic Supplementary Material (ESI) for Nanoscale.

Separator modified by barium titanate with macroscopic polarization electric field for high-performance lithium-sulfur batteries

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Theoretical simulation

The structural optimizations and electronic structure calculations are performed based on density functional theory (DFT) as implemented in the Vienna Ab Initio Simulation Package (VASP) code based on the projector augmented wave (PAW) method with a cutoff energy of 600 eV [1]. The Brillouin zone sampling is carried out using the (3 × 3 × 1) Monkhorst-Pack grids for surface and Gamma for the structure. The convergence tolerance of energy is 1×10^{-5} eV, maximum force is 0.002 eV Å^{-1} and maximum displacement is 0.002 Å [2]. The binding energy of defects was defined as : $E_{bind} = E_{Total} - E_{(BaTiO_3)} - E_{(Li_2S_x)}$, where E_{Total} is the energy of the relevant supercell of Li_2S_x adsorbed with $BaTiO_3$. $E_{(BaTiO_3)}$ is the energy of the relevant supercell of $BaTiO_3$, $E_{(Li_2S_x)}$ is the energy of Li_2S_x The preferential exposure surface of is (001) owing to the smallest surface energy in Table S2.

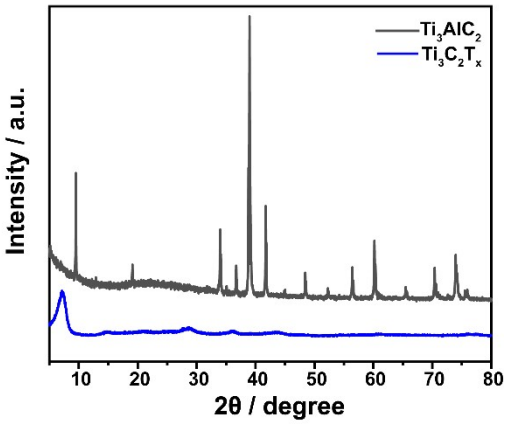

Fig. S1. XRD spectra of the $Ti_3C_2T_x$ and Ti_3AlC_2.

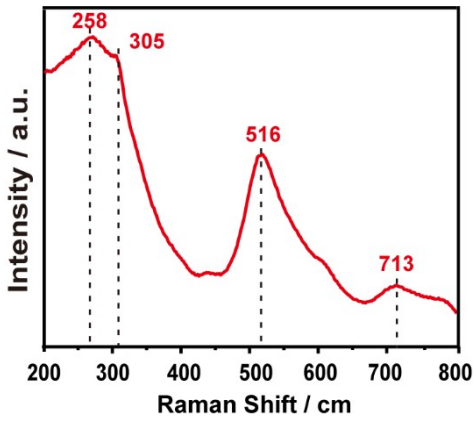

Fig. S2. Raman spectra of the BTO. The band at 305 cm^{-1} was on behalf of the asymmetry of the TiO_6 octahedron.

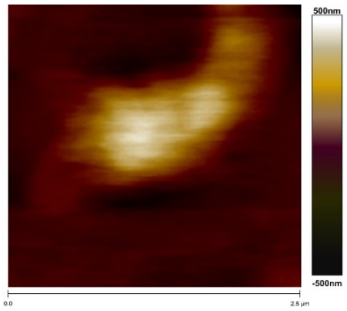

Fig. S3. The BTO topography image obtained by PFM characterization

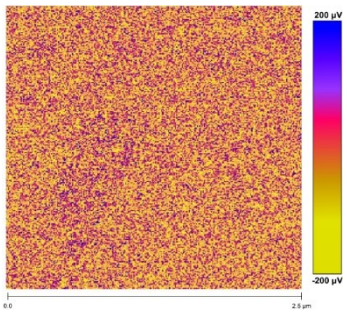

Fig. S4. The BTO amplitude image obtained by PFM characterization

Fig. S5. d_{33} values of the PP/PBTO surface. The front side of PP/PBTO is positively charged, while the reverse side is negatively charged, meaning the electropositivity of PP/PBTO surface.

Fig. S6. d_{33} values of PP/BTO surface

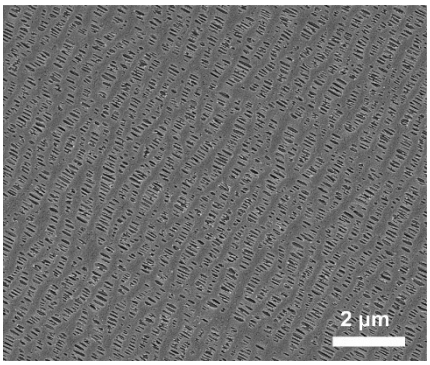

Fig.S7 SEM image of pristine PP

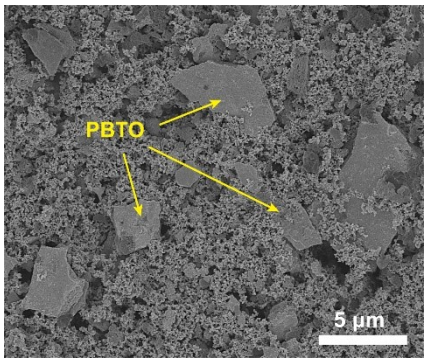

Fig.S8 SEM image of pristine PP/PBTO

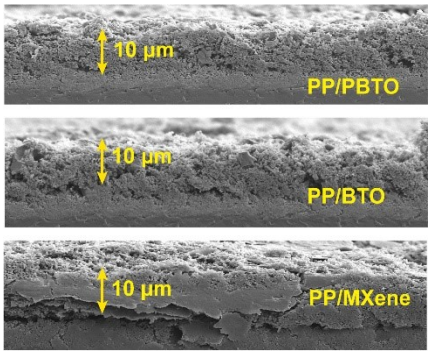

Fig.S9 SEM images for cross sections of PP/PBTO, PP/BTO and PP/MXene

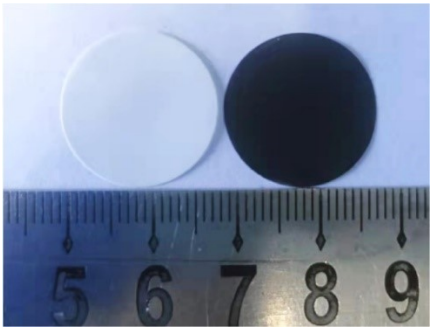

Fig. S10. Photographs of the pristine PP separator and PP/PBTO.

Fig.S11 Contacting angle testing results

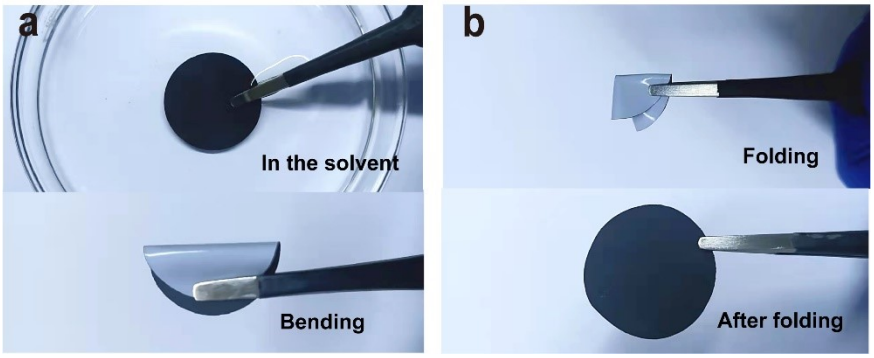

Fig.S12 a) and b) Photographs of PP/PBTO under different stresses.

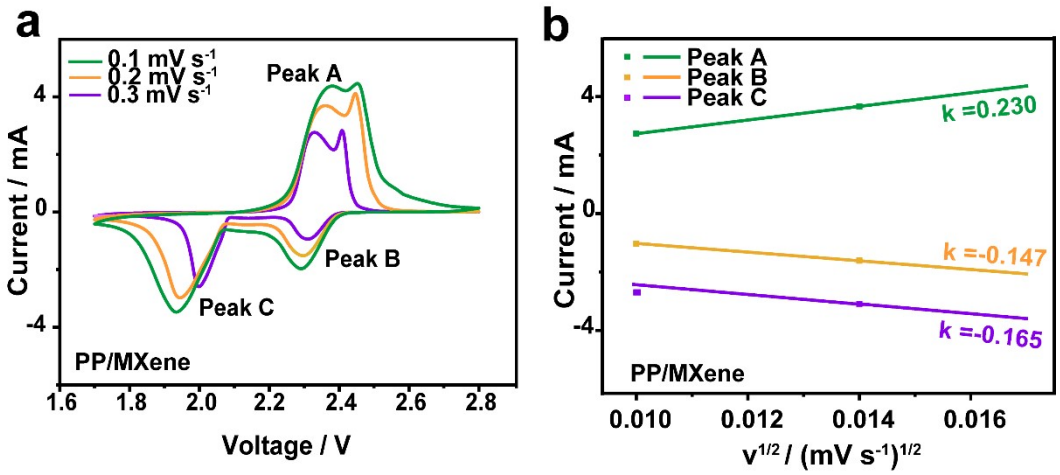

Fig. S13. a) CV curves at scan rates ranging from 0.1 to 0.3 mV/s for the PP/MXene. b)

The slope of the equation is positively related with Li^+ diffusion.

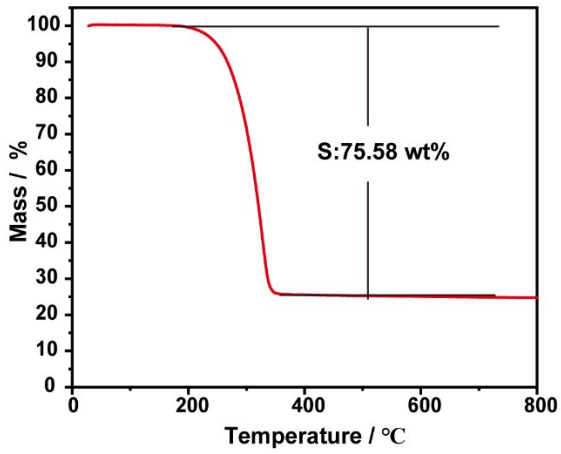

Fig. S14. TGA curve of the S/CNT electrode.

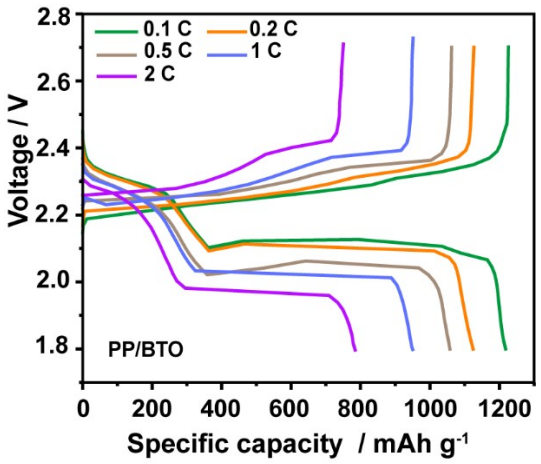

Fig. S15. Discharge-charge curves of the BTO battery at different rates.

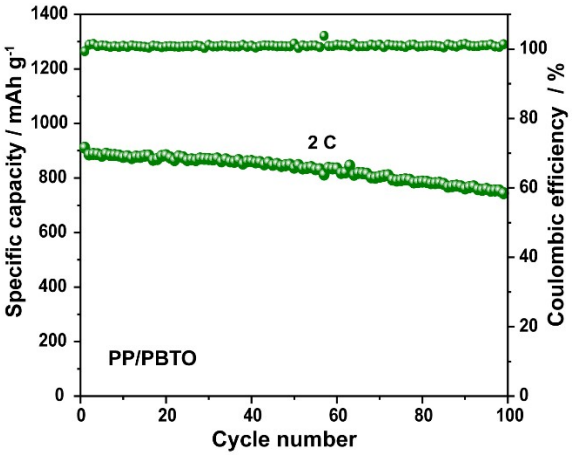

Fig. S16. The PBTO battery at current density of 2 C.

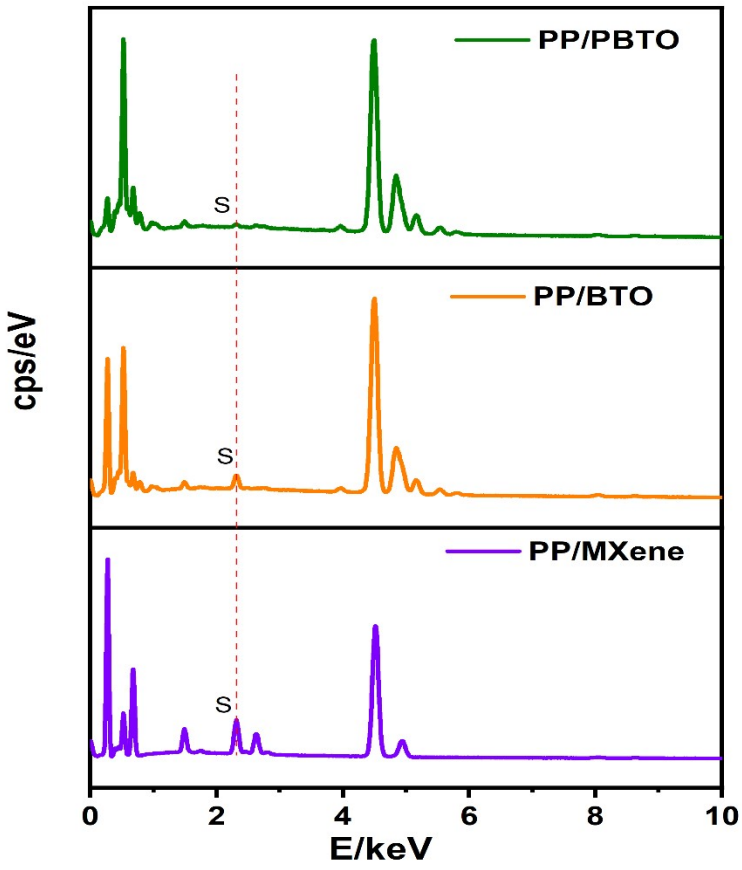

Fig. S17.EDS images of functionalized separators after 100 cycles at 1C.

Table S1. The binding energy of all the structure.

	$BaTiO_3$+Li_2S_4	$BaTiO_3$+Li_2S_6	$BaTiO_3$+Li_2S_8
Before Poling	-2.00 eV	-1.26 eV	-0.77 eV
After Poling	-2.07 eV	-1.50 eV	-0.10 eV

Table S2. The Surface energy of (001), (010) and (100) surface for $BaTiO_3$.

Surface	001	010	100
E(Surf)/eV	-495.2 eV	-471.6 eV	-486.6 eV

Table S3. Diffusion coefficient of Li^+ for the PP/PBTO, PP/BTO and PP/MXene.

$D_{Li^+} \times 10^{-8}(cm^2/s)$	**Peak A**	**Peak B**	**Peak C**
PP/MXene	7.17	3.73	2.92
PP/BTO	12.48	7.12	3.46
PP/PBTO	**14.29**	**10.07**	**3.99**

References

1. G. Kresse and J. Hafner, *Phys Rev B Condens Matter*, 1993, **47**, 558-561.
2. A. E. Mattsson, R. Armiento and T. R. Mattsson, *Phys Rev Lett*, 2008, **101**, 239701; author reply 239702.