

# Oxygen Vacancies in Bismuth Tantalum Oxide to Anchor Polysulfide and Accelerate the Sulfur Evolution Reaction in Lithium–Sulfur Batteries

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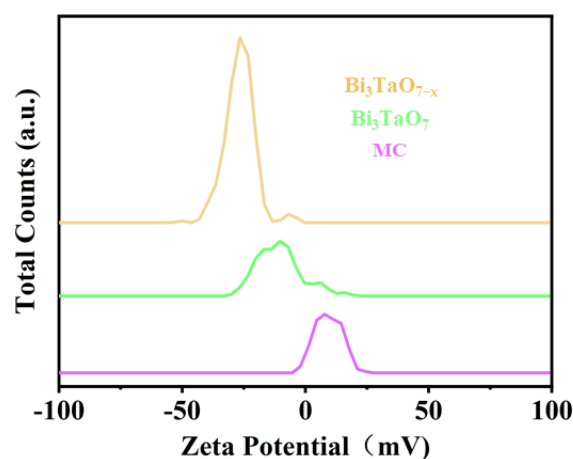


Figure S1. Zeta potentials of the dispersed three samples in water at pH value of 7.0.

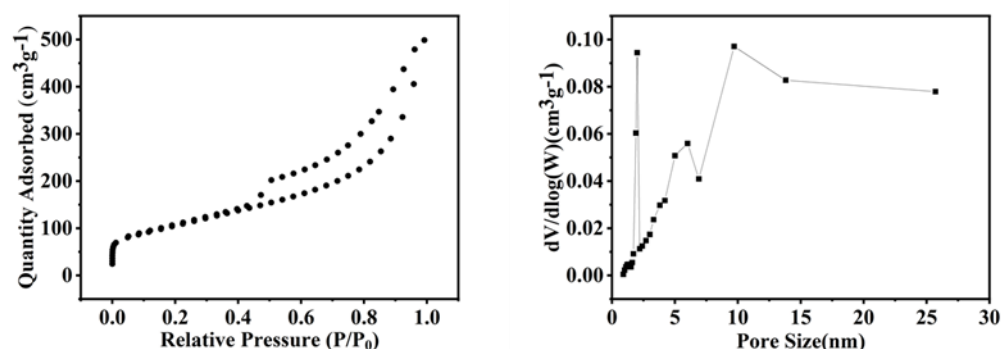
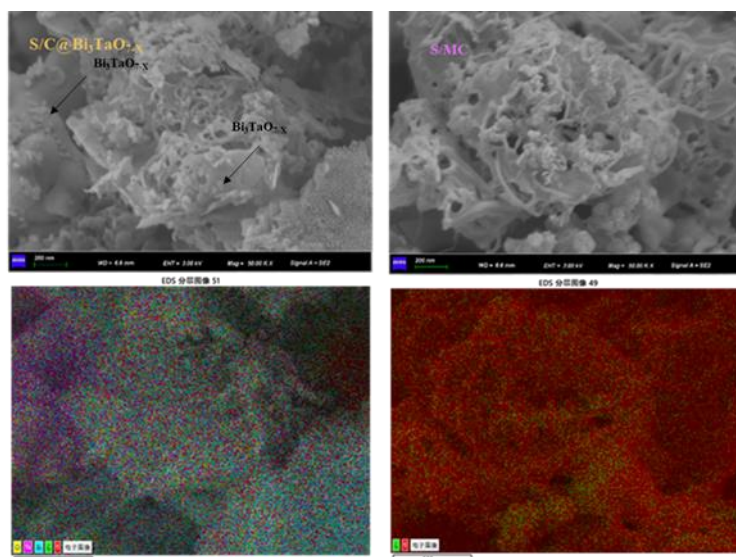
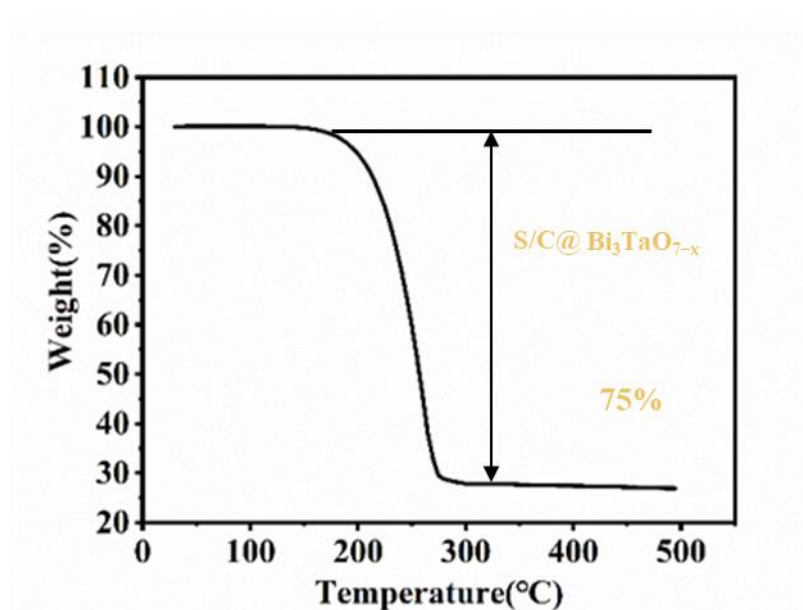


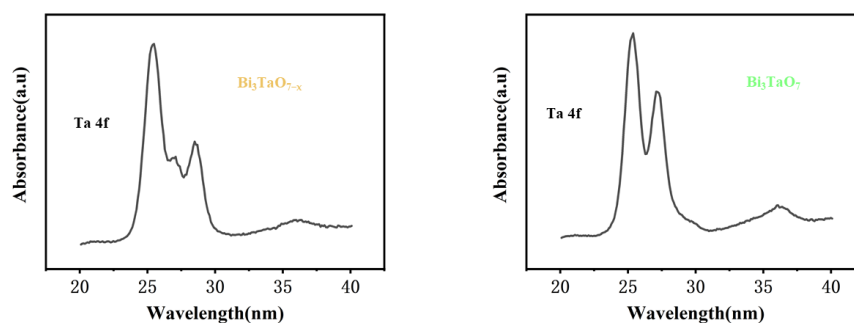
Figure S2. N<sub>2</sub> adsorption-desorption isotherm curves and the pore size distribution of Bi<sub>3</sub>TaO<sub>7-x</sub>.



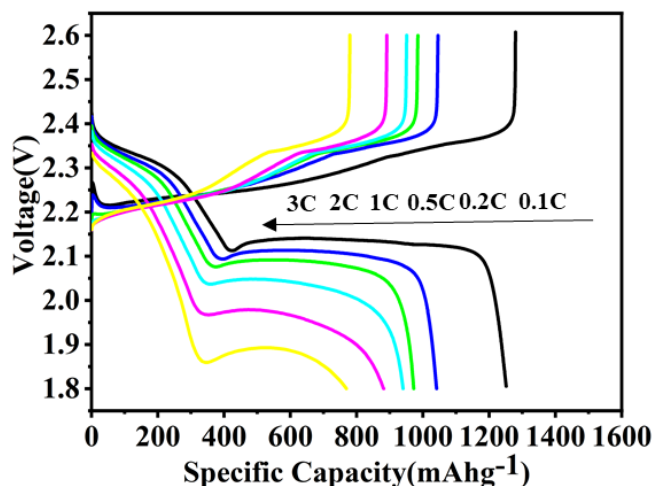
**Figure S3.** Characterization of SEM images and corresponding EDS elemental mappings of S/C and S/C@Bi<sub>3</sub>TaO<sub>7-x</sub>.



**Figure S4.** TGA curve of S/C@Bi<sub>3</sub>TaO<sub>7-x</sub>.



**Figure S5.** Ta 4f for Bi<sub>3</sub>TaO<sub>7</sub> and Bi<sub>3</sub>TaO<sub>7-x</sub>.



**Figure S6.** Multi-rate discharge-charge profiles of S/C@Bi<sub>3</sub>TaO<sub>7-x</sub>.

**Table S1.** The gravimetric energy is calculated based on all active and inactive components, including the packing film, current collectors, and separator.

Parameters	Unit	Value
Sulfur loading	%	80
Carbon content	%	10
Binder content	%	10
Electrolyte/sulfur ratio	$\mu\text{L mg}^{-1}$	3.3
Number of double-sided coated cathode		6
Weight of tab	g	0.28
Weight of the sulfur	g	2.82
Weight of the packing plus pouch foil	g	2.5
Weight of the anode	g	3.6
Weight of the cathode	g	4.70
Weight of the separator	g	0.64
Weight of electrolyte	g	9.30
Total weight	g	21.02
Energy of cell	Wh	6.3
Energy Density	Wh kg <sup>-1</sup>	299

**Table S2.** Comparative table of Li-S pouch cell performance with recently reported works.

S loading (mg cm <sup>-2</sup> )	Energy density (W h kg <sup>-1</sup> )	E/S ratio ( $\mu\text{L mg}^{-1}$ )	Areal capacity (mA h cm <sup>-2</sup> )	Capacity retention rate (%)	Cycle	References
4.0	206	6.0	4.8	~88	40	[1]
4.1	150	4.5	3.3	51	66	[2]
4.9	301	4.0	6.5	89	30	[3]
5.0	118	7.0	4.5	~77	50	[4]
6.0	317	4.0	7.2	74	80	[5]
6.1	301.4	3.0	7.1	81	23	[6]
6.5	299	2.5	5.9	83	10	[7]
13.6	303	2.4	11.0	78	30	[8]
<b>9.6</b>	<b>299.0</b>	<b>3.3</b>	<b>10.20</b>	<b>54</b>	<b>53</b>	<b>This work*</b>

## References

1. Zhao, M.; Chen, X.; Li, X. Y.; Li, B. Q.; Huang, J. Q. An organodiselenide comediator to facilitate sulfur redox kinetics in lithium–sulfur batteries. *Adv. Mater.* **2021**, *33*, 2007298.
2. He, J.; Bhargava, A.; Manthiram, A. High-Energy-Density, Long-Life Lithium–Sulfur Batteries with Practically Necessary Parameters Enabled by Low-Cost Fe–Ni Nanoalloy Catalysts. *ACS Nano* **2021**, *15*, 8583–8591.
3. Huang, Y.; Shaibani, M.; Gamot, T. D.; Wang, M.; Jovanović, P.; Cooray, D.; Majumder, M. A saccharide-based binder for efficient polysulfide regulations in Li-S batteries. *Nat. Commun.* **2021**, *12*, 1–15.
4. Luo, L.; Li, J.; Yaghoobnejad Asl, H.; Manthiram, A. In-situ assembled VS<sub>4</sub> as a polysulfide mediator for high-loading lithium–sulfur batteries. *ACS Energy Lett.* **2020**, *5*, 1177–1185.
5. Zhao, C.; Xu, G. L.; Yu, Z.; Zhang, L.; Hwang, I.; Mo, Y. X.; Zhao, T. A high-energy and long-cycling lithium–sulfur pouch cell via a macroporous catalytic cathode with double-end binding sites. *Nat. Nanotechnol.* **2021**, *16*, 166–173.
6. Zhang, X. Q.; Jin, Q.; Nan, Y. L.; Hou, L. P.; Li, B. Q.; Chen, X.; Zhang, Q. Electrolyte Structure of Lithium Polysulfides with Anti-Reductive Solvent Shells for Practical Lithium–Sulfur Batteries, *Angew. Chem. Int. Ed.* **2021**, *60*, 15503–15509.
7. Qi, C.; Li, Z.; Wang, G.; Yuan, H.; Chen, C.; Jin, J.; Wen, Z. Microregion Welding Strategy Prevents the Formation of Inactive Sulfur Species for High-Performance Li-S Battery, *Adv. Energy Mater.* **2021**, *11*, 2102024.
8. Wang, X.; Yang, Y.; Lai, C.; Li, R.; Xu, H.; Tan, D. H.; Loh, K. P. Dense-Stacking Porous Conjugated Polymer as Reactive-Type Host for High-Performance Lithium Sulfur Batteries, *Angew. Chem. Int. Ed.* **2021**, *60*, 11359–11369.