

Supporting Information

Pyrochlore Phase $\text{Ce}_2\text{Sn}_2\text{O}_7$ via Atomic-Confined Strategy for Reversible Lithium storage

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1. Experimental Section

1.1 Preparation of $\text{Ce}_2\text{Sn}_2\text{O}_7$

All chemicals were purchased from Alladin and were used as received without purification. The precursor of the new compound $\text{Ce}_2\text{Sn}_2\text{O}_7$ was prepared by a hydro-thermal method. In a typical procedure, 3 mmol Na_2SnO_3 , 1.5 mmol $\text{Ce}(\text{NO}_3)_3$ and 1g NaOH were dissolved in 20ml deionized water to obtain an aqueous solution. The solution was thoroughly mixed by vigorous stirring. Then the resulting slurry was transferred into an autoclave, and hydro-thermal treated at 200°C for 24 h. After naturally cooling, the resultant precursor was filtered and dried at 80°C . The as-synthesized precursors were subsequently heated at 400°C for 2 h to produce the final products.

1.2 Sample Characterization

Raman spectra were collected on a Thermal Dispersive Spectrometer using a laser with an excitation wavelength of 532 nm at a laser power of 10 mW. XPS experiments were carried out on an RBD upgraded PHI-5000C ESCA system (Perkin Elmer) with Mg $K\alpha$ radiation ($h\nu = 1253.6$ eV). XRD patterns were obtained with a Bruker D8 advance diffractometer operating with Cu $K\alpha$ radiation. The morphologies of the samples were observed on a JEOL-JEM 2100F transmission electron microscope (TEM) (100 kV) and a Hitachi S-4800 field emission scanning electron microscope (FE-SEM) (5 kV).

1.3 Electrode preparation and electrochemical testing

Electrochemical measurements were performed using coin cells assembled in an argon-filled glove box (German, M. Braun Co., [O₂] b 1 ppm, [H₂O] b 1 ppm). The composite electrodes were made of the active material powder (80 wt%), acetylene black (10 wt%) and a polyvinylidene fluoride (PVDF) binder (10 wt%) homogeneously mixed in N-methyl pyrrolidinone (NMP) solvent and then coated uniformly on a copper foil. Pure lithium foil was used as a counter electrode. The electrolyte consisted of a solution of 1 M LiPF₆ in ethylene carbonate and dimethyl carbonate (EC + DMC + EMC) (1:1:1 in volume). Galvanostatic cycling of the assembled cells was carried out using a Land CT2001A tester (Wuhan, China) between cutoff voltages of 3.0 and 0.01 V at room temperature. A CHI760e electrochemical workstation was used for cyclic voltammetry measurements with a potential range between 0.01 and 3.0 V at a scan rate of 0.1 mV s⁻¹.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) of $\text{Ce}_2\text{Sn}_2\text{O}_7$

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ce1	0.00000	0.00000	0.00000	0.001 (3)*
Sn1	0.50000	0.50000	0.50000	0.01267*
O1	0.12500	0.12500	0.12500	0.00671*
O2	0.380 (3)	0.12500	0.12500	0.03166*

Table S2. Summary of the crystal parameters of SnO_2 , CeO_2 , and $\text{Ce}_2\text{Sn}_2\text{O}_7$.

Compound	Crystal System	Z	Packing factor (%)
SnO_2	Tetragonal	2	65.7
CeO_2	Cubic	4	62.5
$\text{Ce}_2\text{Sn}_2\text{O}_7$	Cubic	8	56.8

Table S3. Comparison of electrochemical performances for Tin-based anodes.

Anodes	Capacity@0.1 A g^{-1} (mA h g^{-1})	Rate capacity (mA h g^{-1})	References
Black (Sn,Ti) O_2	583 (100 cycles)	335 (5 A g^{-1})	ref 12
Ordered network of interconnected SnO_2	564 (100 cycles)	300 (4.7 A g^{-1})	ref S1
$\text{SnO}_2\text{-Fe}_2\text{O}_3\text{-Li}_2\text{O}$	1150 (100 cycles)	747 (5 A g^{-1})	ref 20
Ag- SnO_2/NiO	826 (500 cycles)	721 (5 A g^{-1})	ref S2
Zn_2SnO_4	580 (50 cycles)	none	ref S3
$\text{Ce}_2\text{Sn}_2\text{O}_7$	631 (330 cycles)	384 (5 A g^{-1})	This work

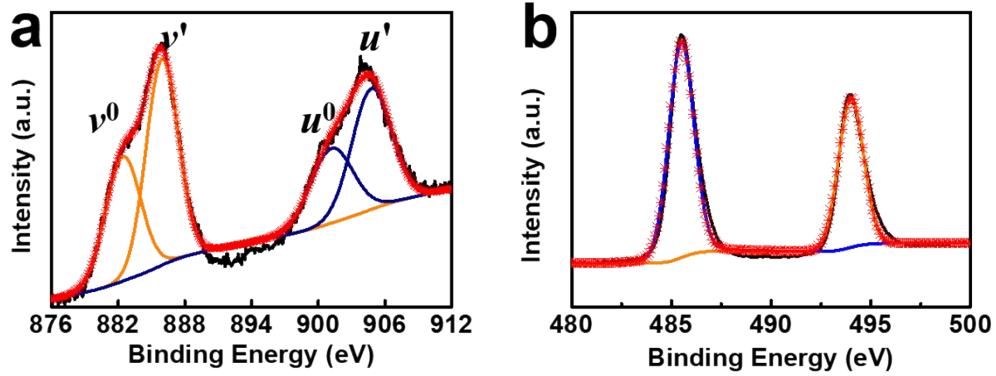


Figure S1. XPS spectra: (a) Ce 3d, (b) Sn 3d, of $\text{Ce}_2\text{Sn}_2\text{O}_7$.

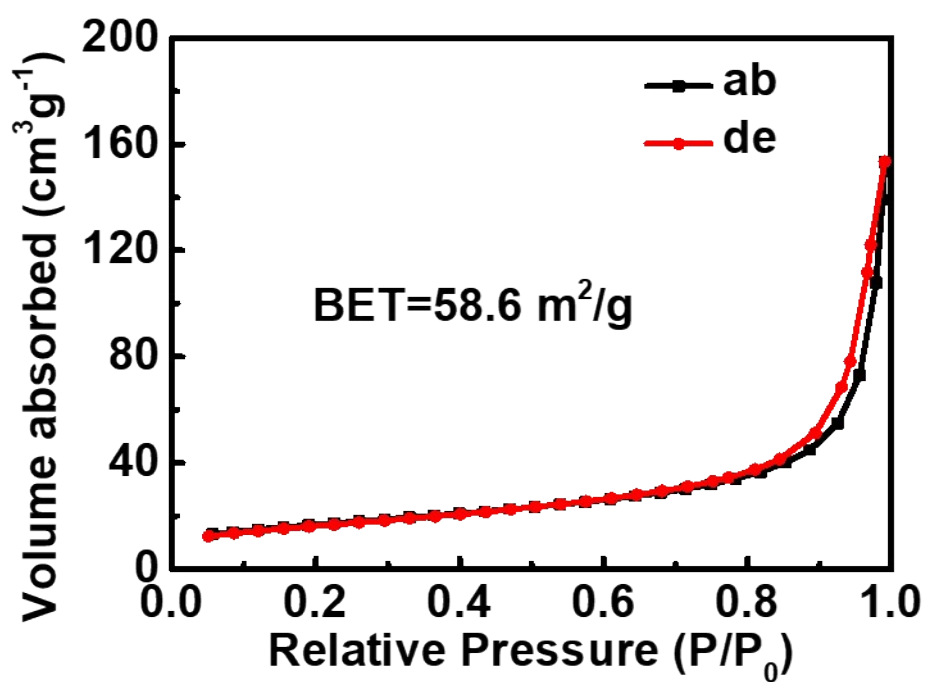


Figure S2. N₂ adsorption–desorption isotherm of Ce₂Sn₂O₇.

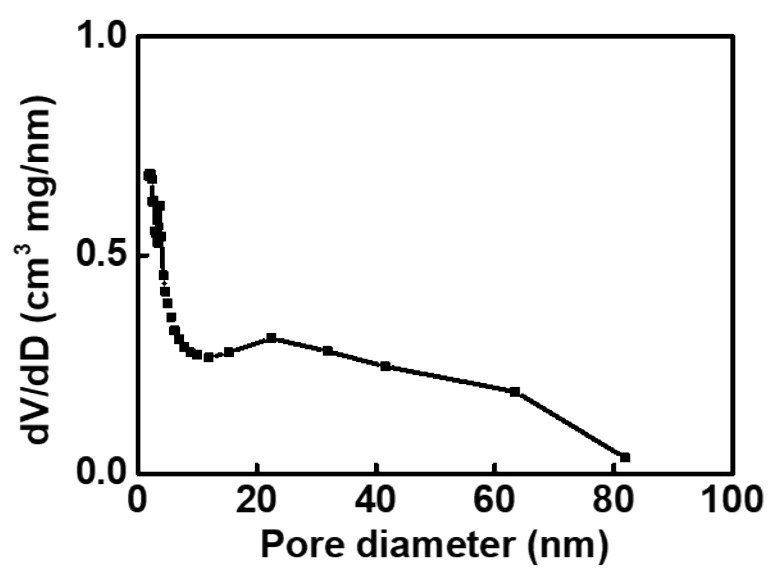


Figure S3. Pore size distribution of Ce₂Sn₂O₇.

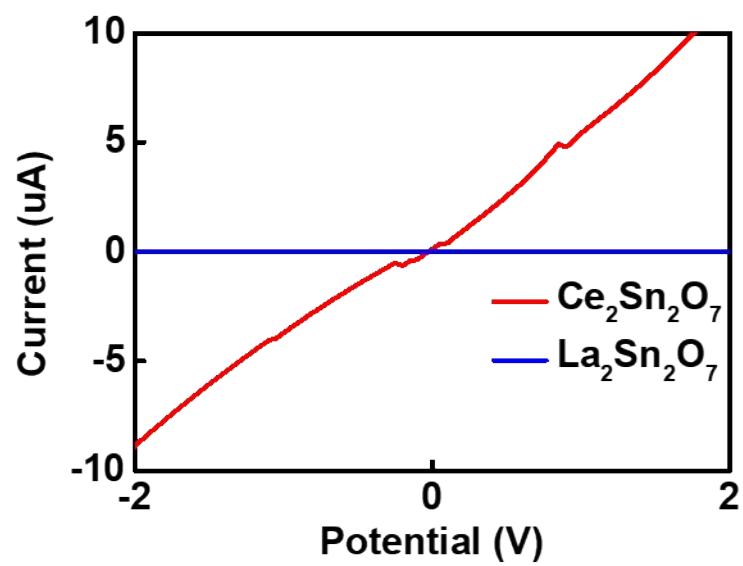


Figure S4. Room-temperature I-V characteristics of compressed pellets of La₂Sn₂O₇ and Ce₂Sn₂O₇.

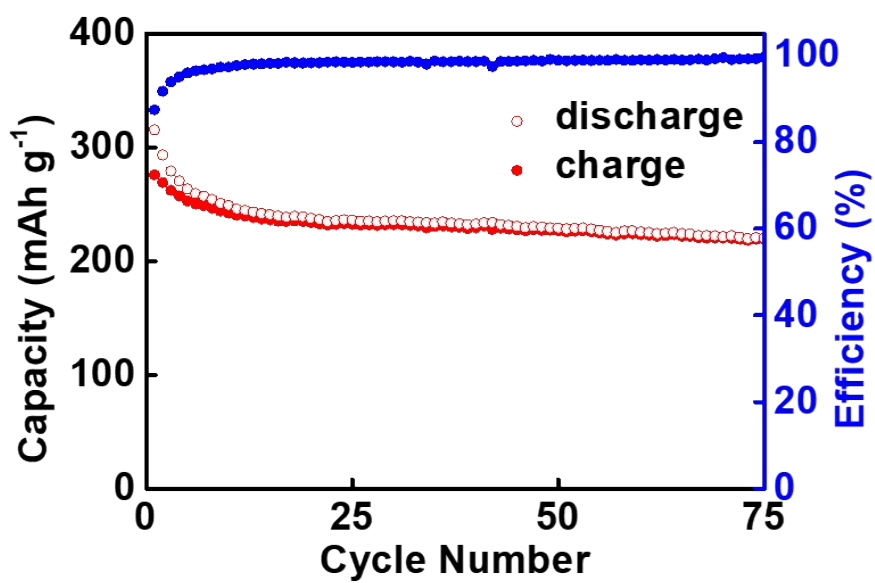


Figure S5. Cycle performance of CeO₂ electrode at a current density of 0.1 A/g.

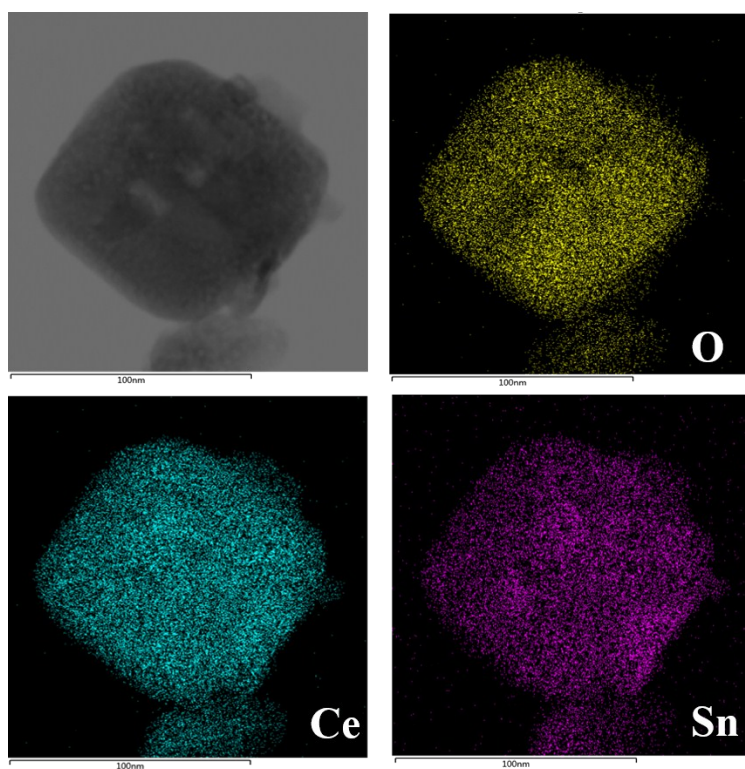


Figure S6. Elemental mapping images of $\text{Ce}_2\text{Sn}_2\text{O}_7$ after 100 cycles.

[S1] V. Etacheri, G. A. Seisenbaeva, J. Caruthers, G. Daniel, J. M. Nedelec, V. G. Kessler, V. G. Poi, *Adv. Energy Mater.* 2015, 5, 1401289.

[S2] C. Kim, J. W. Jung, K. R. Yoon, D. Y. Youn, S. Park, I. D. Kim, A high-capacity and long-cycle-life lithium-ion battery anode architecture: silver nanoparticle-decorated SnO₂/NiO nanotubes. *ACS nano*, 2016, 10, 11317-11326.

[S3] A. Rong, X. P. Gao, G. R. Li, T. Y. Yan, H. Y. Zhu, J. Q. Qu, D. Y. Song, Hydrothermal synthesis of Zn₂SnO₄ as anode materials for Li-ion battery. *The Journal of Physical Chemistry B*, 2006, 110, 14754-14760.