Oxygen defects-engineered build $Zn_2P_2O_{7-y}$ as anode materials for Lithium-ion batteries

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Physical measurements

The XRD patterns were tested using a Bruker D2 X-ray powder diffractometer equipped with a Cu Kα radiation source (tube voltage = 30 kV, λ = 1.5418 Å). High-resolution transmission electron microscopy (HRTEM, ZEISS Libra 200 FE) was used to study the morphology of $Zn_2P_2O_{7-y}$. The Electron paramagnetic resonance (EPR) was using Bruker A 300 spectrometer, and the operating frequency was about 9.4 GHz. Thermogravimetric analysis (TGA) was measured using an SDT-Q600 thermal analyzer at a heating rate of 10 ℃ min^{-1} in air. Energy Dispersive Spectrometer (EDS) was using EDAX ELECT PIUS (15 kV, 60 s).

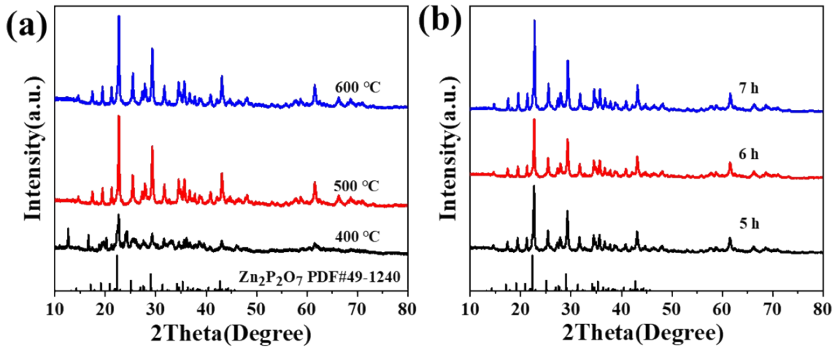

Fig. S1. the XRD patterns of $Zn_2P_2O_{7-y}$ synthesized with different calcined temperature and time.

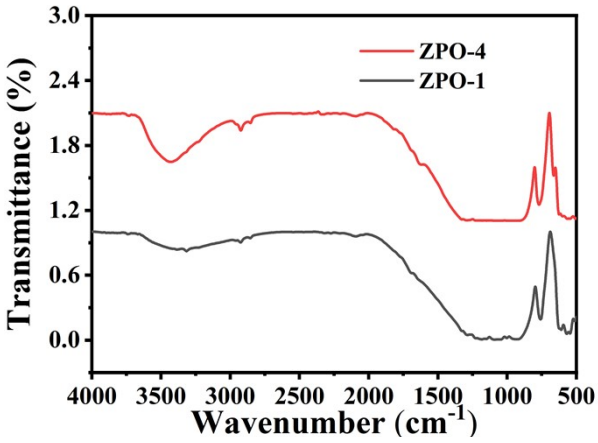

Fig.S2 FTIR spectra of ZPO-1 and ZPO-4.

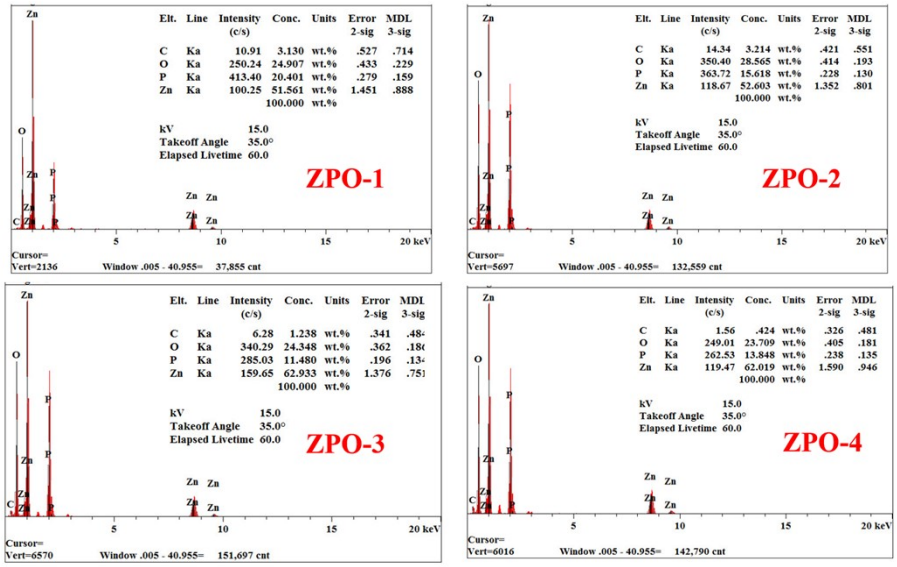

Fig.S3 EDX analysis of ZPO-1, ZPO-2,ZPO-3 and ZPO-4, respectively.

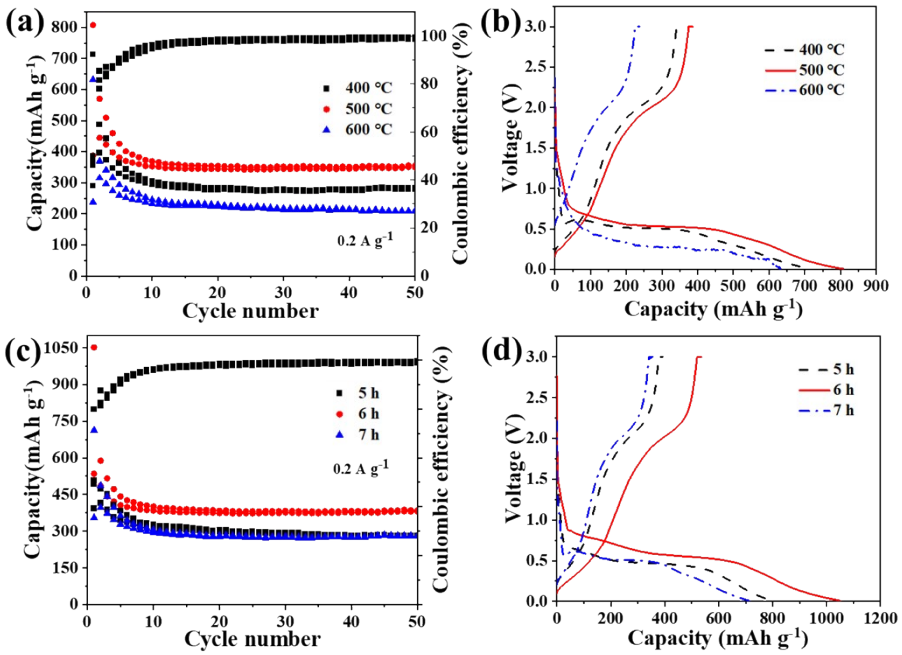

Fig. S4 (a) Cycle performance of $Zn_2P_2O_{7-y}$ synthesized at different calcination temperatures at 0.2 A g^{-1} (b) Initial charge-discharge curves of $Zn_2P_2O_{7-y}$ synthesized at different calcination temperature.(c) Cycle performance of $Zn_2P_2O_{7-y}$ synthesized for 500 ℃ at different calcination times at 0.2 A g^{-1} (d) Initial charge-discharge curves of $Zn_2P_2O_{7-y}$ synthesized for 500 ℃ at different calcination times.

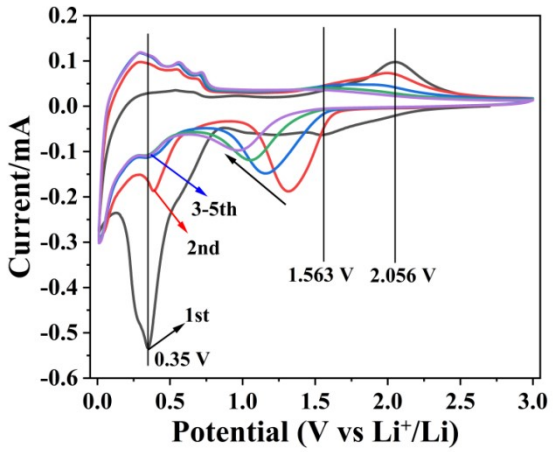

Fig. S5 Cyclic voltammetry curves of ZPO-1 for 1-5 cycles.

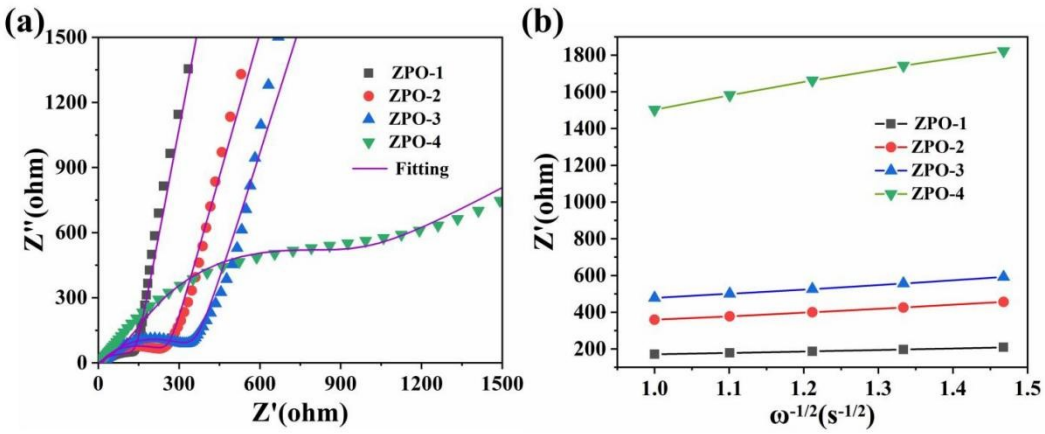

Fig. S6 Samples of ZPO-1, ZPO-2, ZPO-3 and ZPO-4 (a) AC impedance and (b) equivalent circuit fitting curve.

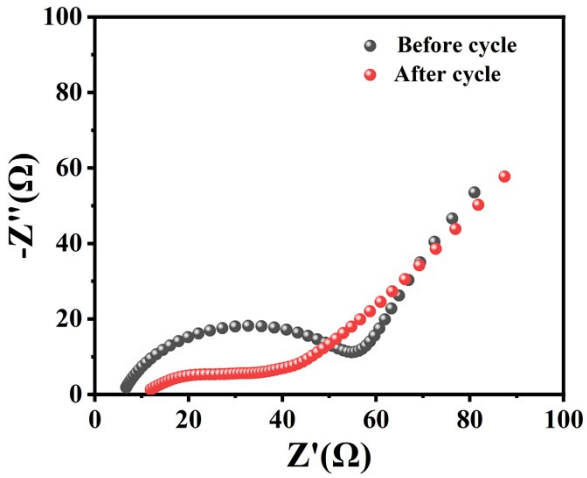

Fig. S7 EIS of the ZPO-1 electrodes before the cycling test and after 500 cycles.

Table S1. The peaks appear in positions corresponding to the vibrations of the groups of ZPO-1.

Absorption bands	Attribution
3400 cm^{-1}	The stretching of O-H of water in air
1290 cm^{-1}	The stretching vibrations of *vs*(O-P-O)
1100 cm^{-1}	The stretching vibrations of *vs*(O-P-O)

945 cm^{-1}	The asymmetric and symmetric stretches of PO_3 terminal groups
763 cm^{-1}	The stretching vibration of P-O-P bridges
624 cm^{-1}	The fundamental frequency of the $[PO_4]^{3-}$ group
576 cm^{-1}	The asymmetric P-O-P bridge

Table S2 The lattice parameter of $Zn_2P_2O_{7-y}$ by different calcination atmosphere.

lattice parameter	ZPO-1	ZPO-2	ZPO-3	ZPO-4
a	4.97	4.95	4.92	4.90
b	13.39	13.29	13.16	13.15
c	16.46	16.43	16.38	16.36
Vol	1089.30	1070.66	1064.90	1060.44

Note: ZPO-1(Argon-hydrogen mixture), ZPO-2(Argon), ZPO-3(Vacuo), ZPO-4(Air)

Table S3 The atomic ratio of C/O/P/Zn estimated from EDX data of ZPO-1.

Compound	Element Percentage(C:O:P:Zn) %
ZPO-1	3.13 : 24.91 : 20.40 : 51.56
ZPO-2	3.21 : 28.56 : 15.62 : 52.61
ZPO-3	1.24 : 24.35 : 11.48 : 62.29
ZPO-4	0.42 : 23.71 : 13.85 : 62.02

Table S4 The rare values of $Zn_2P_2O_{7-y}$ by different calcination atmosphere (mAh g^{-1})

Current density	ZPO-1	ZPO-2	ZPO-3	ZPO-4
0.2 A g^{-1}	1178.4	749.1	901.3	911.2
0.5 A g^{-1}	335.2	263.1	250.9	248.6

1 A g^{-1}	261.2	200.3	193.9	185.3
2 A g^{-1}	192.3	146.6	143.9	129.4
5 A g^{-1}	73.1	66.1	61.6	51.3
1 A g^{-1}	251.7	177.5	159.7	150.3
0.5 A g^{-1}	284.6	238.6	198.0	193.6
0.2 A g^{-1}	364.1	297.5	221.5	218.6
1 A g^{-1}	277.2	207.8	165.3	152.5

Table S5 Cycling capacityof $Zn_2P_2O_{7-y}$ by different calcination atmosphere at 1 A g^{-1}.

	ZPO-1	ZPO-2	ZPO-3	ZPO-4
Initial discharge capacity	633.7	608.7	293.0	251.8
Initial charge capacity	209.7	179.2	87.8	82.3
Discharge capacity after 1200 cycles	260.6	211.2	158.0	103.2 (600 cycles)
Charge capacity after 1200 cycles	260.4	211.0	157.7	103.0 (600 cycles)
Capacity retention rate	41.1%	34.7%	53.9%	40.9 %

Table S6 AC impedance of $Zn_2P_2O_{7-y}$ by different calcination atmosphere.

sample	Rs(Ω)	Rct(Ω)	бw($cm^2s^{-0.5}$)	D_{Li}^+(cm^2 s^{-1})
ZOP-1	2.13	157.5	65.4	8.53×10^{-14}
ZOP-2	8.45	270.5	162.9	1.26×10^{-14}
ZOP-3	16.7	364.5	197.6	9.28×10^{-15}
ZOP-4	10.12	1492.0	914.5	1.18×10^{-15}