Photochromic zinc-based coordination polymer for Li-ion batteries anode with higher capacity and stable cycling stability

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Table S1. Crystal Data and Structure Refinements for Zn-BCP.

Complexes	**Zn-BCP**
Empirical Formula	$C_{21}H_{12}NO_7Zn$
Formula weight	455.71
Crystal system	Triclinic
Space group	*P*-1
a (Å)	8.7799(7)
b (Å)	9.6790(7)
c (Å)	12.5229(11)
α (°)	109.152(7)
β (°)	96.773(7)
γ (°)	99.480(6)
V (Å^3)	974.54(14)
Z	2
Dc (g/ cm^3)	1.635
μ(Mo Kα) (mm^{-1})	1.309
F(000)	486
Collected reflections	9196
Independent reflections	3324 (0.041)
Goodness-of-fit on F^2	1.059
$R_1{}^a$, $wR_2{}^b$ ($I>2\sigma(I)$)	0.0507, 0.1377
$R_1{}^a$, $wR_2{}^b$ (all data)	0.0641, 0.1475

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) for Zn-BCP

Bonds	**Dist. (Å)**	**Bonds**	**Dist. (Å)**
Zn1—O1	1.956(3)	Zn1—O4	1.976(3)
Zn1—O5	1.980(3)	Zn1—O7	2.020(3)
Angle	**(°)**	**Angle**	**(°)**
O1—Zn1—O4	113.19(13)	O1—Zn1—O5	105.78(13)
O4—Zn1—O5	100.62(14)	O1—Zn1—O7	127.20(14)
O4—Zn1—O7	105.86(13)	O5—Zn1—O7	100.21(13)

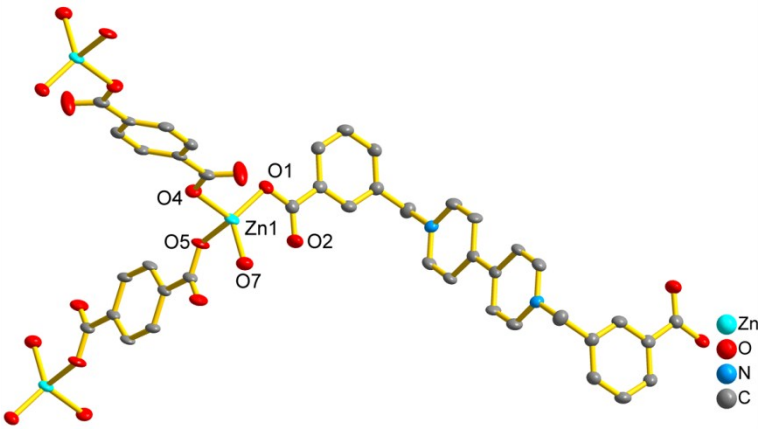


Figure S1. Coordination environment of Zn^{2+} in complex Zn-BCP.

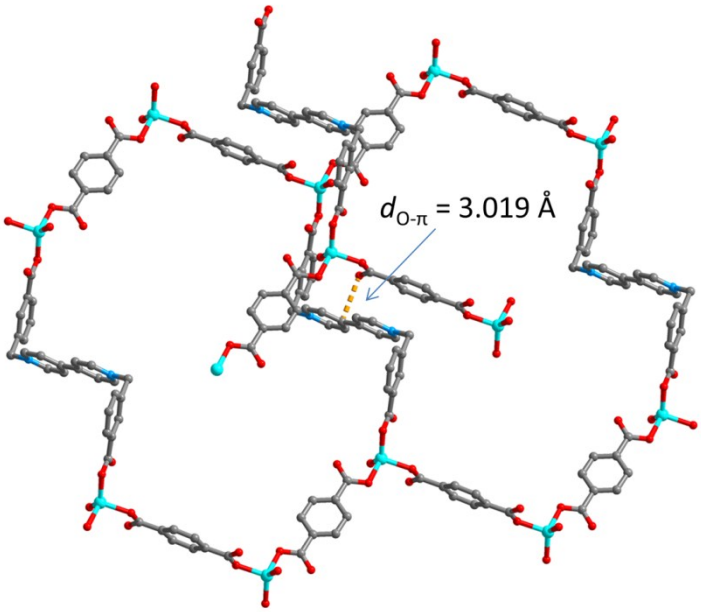


Figure S2. The interactions between carboxylate groups of PTA^{2-} ligand and viologen moiety of bcbpy ligand.

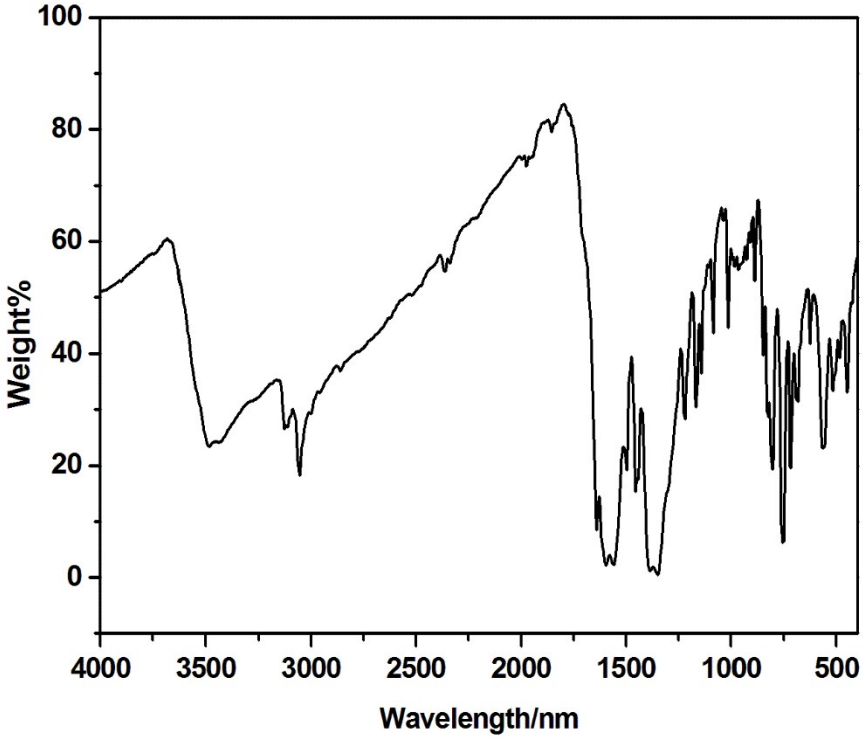


Figure S3. The IR spectrum of Zn-BCP.

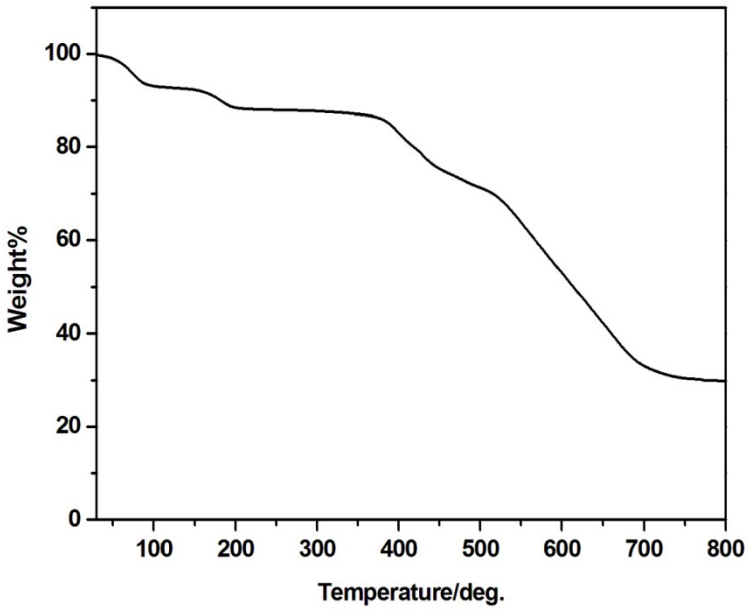


Figure S4. TGA data of the Zn-BCP.

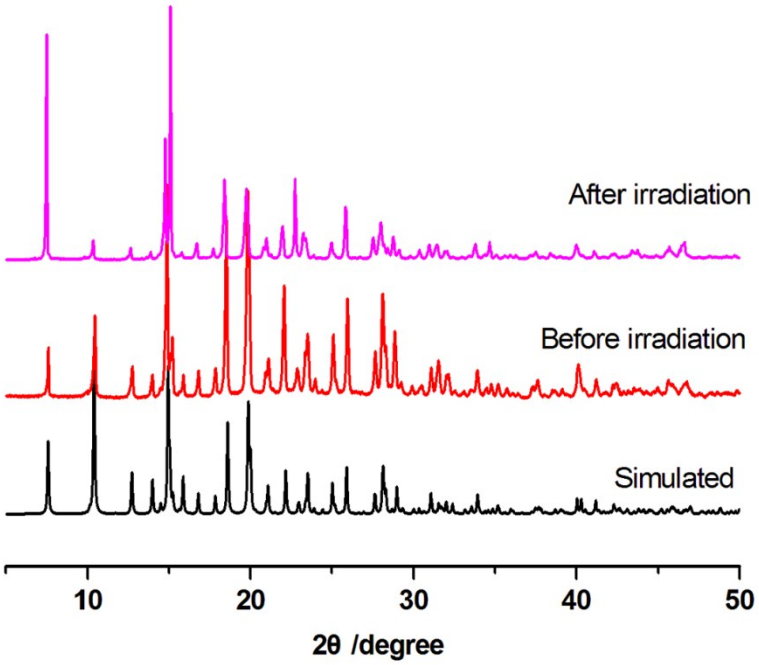


Figure S5. PXRD patterns of Zn-BCP before and after irradiation.

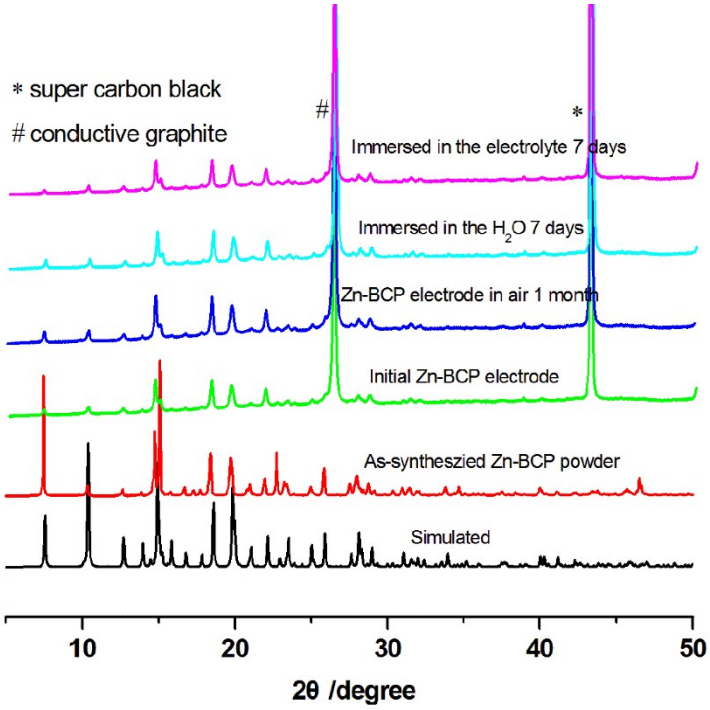


Figure S6. PXRD patterns of the Zn-BCP electrode and immersed in different solvents.

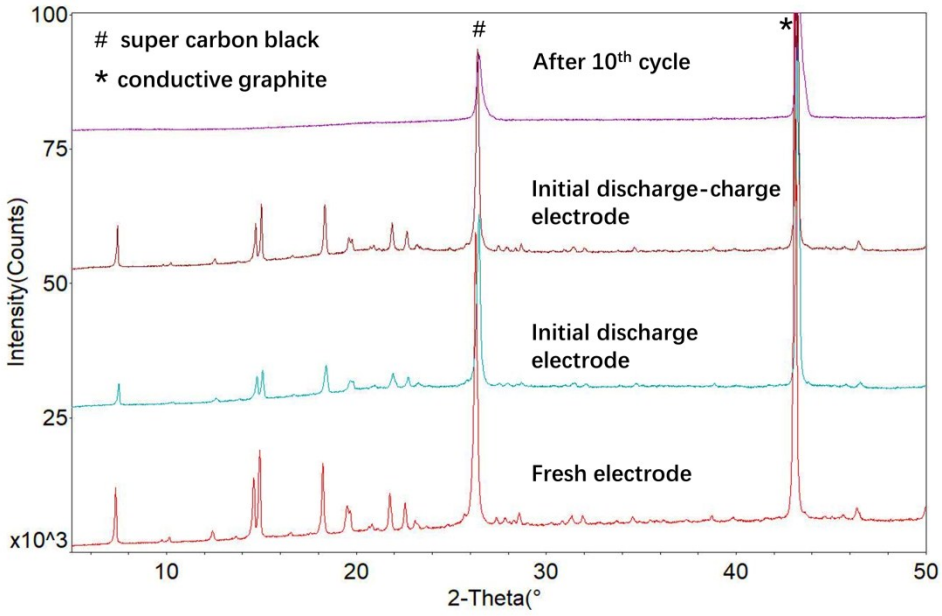


Figure S7. PXRD patterns of the Zn-BCP electrode after 1 and 10 cycles performed.

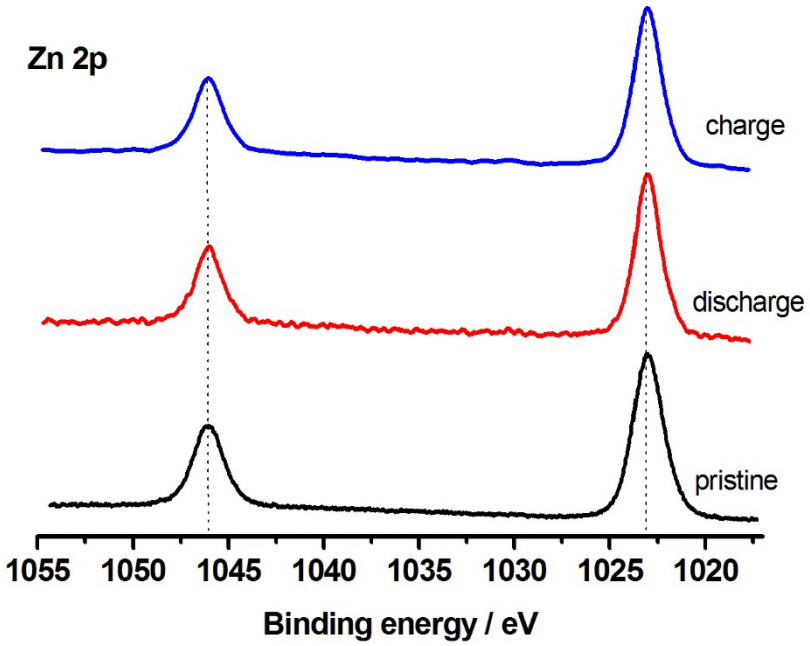
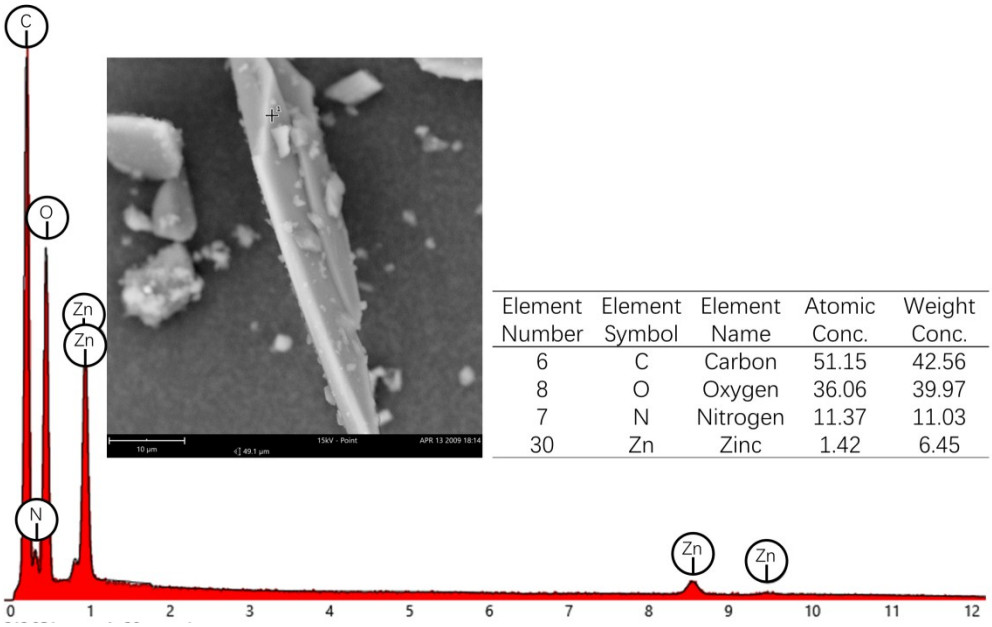


Figure S8. XPS core level spectra of Zn in Zn-BCP electrode.



Element Number	Element Symbol	Element Name	Atomic Conc.	Weight Conc.
6	C	Carbon	51.15	42.56
8	O	Oxygen	36.06	39.97
7	N	Nitrogen	11.37	11.03
30	Zn	Zinc	1.42	6.45

Figure S9. EDS spectrum of Zn-BCP.