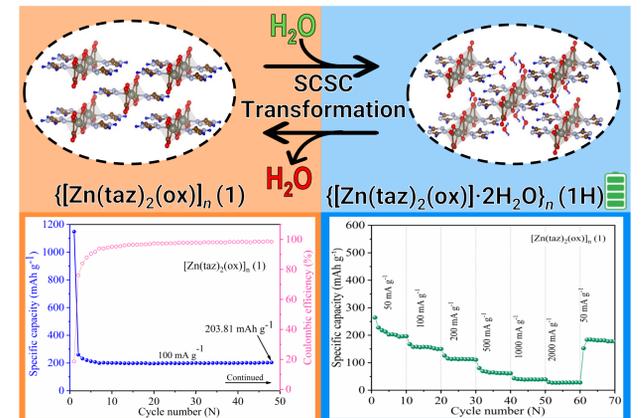


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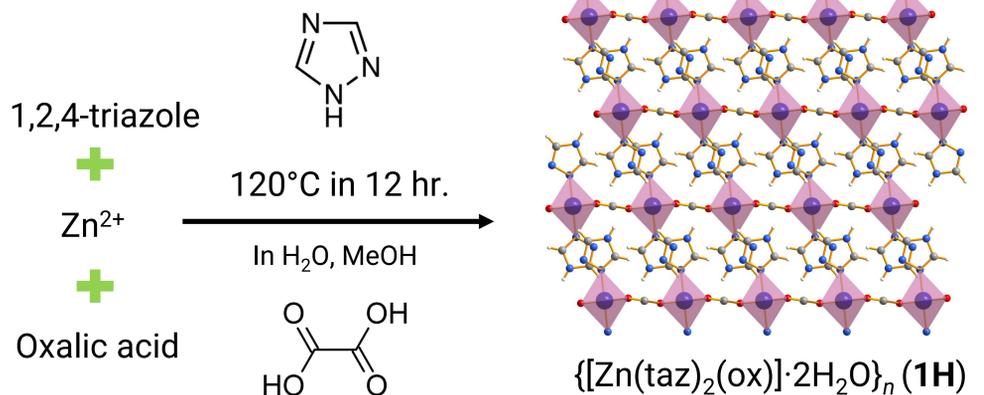
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**Abstract:** A new one-dimensional Zn(II) coordination polymer (CP),  $\{[\text{Zn}(\text{taz})_2(\text{ox})]\cdot 2\text{H}_2\text{O}\}_n$ , [taz = 1,2,4-triazole, ox<sup>2-</sup> = oxalate], C2/m, (1H), was successfully synthesized by solvothermal method. Complex 1H underwent reversible *single-crystal to single-crystal* (SCSC) transformation toward a new coordination polymer,  $[\text{Zn}(\text{taz})_2(\text{ox})]_n$ , I2/m, (1), upon dehydration/rehydration. The electrochemical performance of 1 has been being investigated for use as anode material in lithium-ion batteries. Specific capacity at 100 mA g<sup>-1</sup> after 49 cycles is found to be 203.81 mAh g<sup>-1</sup>.

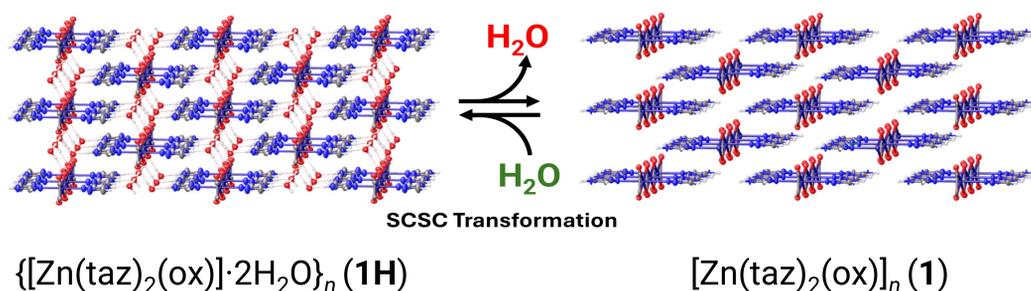


## Methodology

### 1. Synthesis of Zn-CP

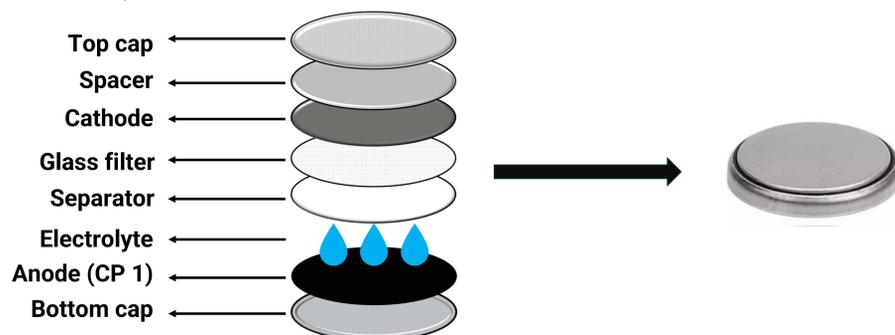


### 2. SC-SC Transformation



### 3. Zn-CP (1) for Li-ion Batteries Anode

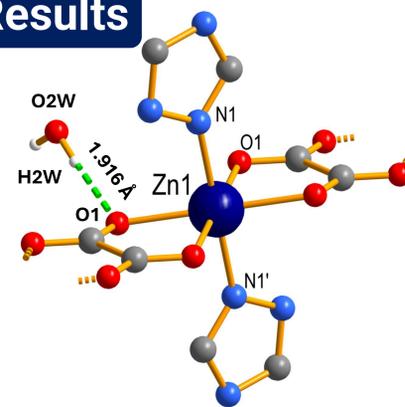
\*Electrolyte = 1.0 mol/L LiPF<sub>6</sub> dissolved in ethylene carbonate : dimethyl carbonate (EC:DMC, 1:1 v/v)



## Conclusion

- The novel 1D CP,  $\{[\text{Zn}(\text{taz})_2(\text{ox})]\cdot 2\text{H}_2\text{O}\}_n$  (1H), was successfully synthesized and demonstrated a reversible transformation into  $[\text{Zn}(\text{taz})_2(\text{ox})]_n$  (1) through the dehydration or rehydration process.
- $[\text{Zn}(\text{taz})_2(\text{ox})]_n$  (1) exhibits properties suitable for application as an anode material in Li-ion batteries.

## Results



### Single-Crystal X-ray Diffraction

Table 1: Crystallographic Information for 1H and 1.

Identification	1H	1
Empirical formula	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>6</sub> Zn	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>4</sub> Zn
Formula weight	325.55	291.54
Crystal system	monoclinic	monoclinic
Space group	C2/m	I2/m
a/Å	14.9839(9)	5.4559(4)
b/Å	7.4906(5)	6.3727(8)
c/Å	5.5064(2)	12.955(2)
β/°	95.045(4)	94.951(7)

Figure 1. Illustrations of an extended asymmetric unit of 1H showing the coordination environment around Zn(II).

### Powder X-Ray Diffraction & FT-IR Spectroscopy

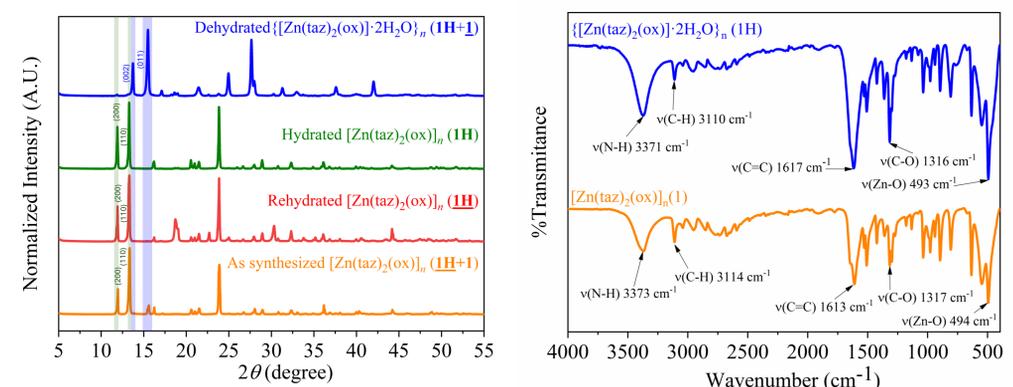


Figure 2. (a) PXRD patterns of Zn-CP 1H upon dehydration/rehydration. (b) The IR spectra of the Zn-CP 1, and Zn-CP 1H.

## Electrochemical Performance

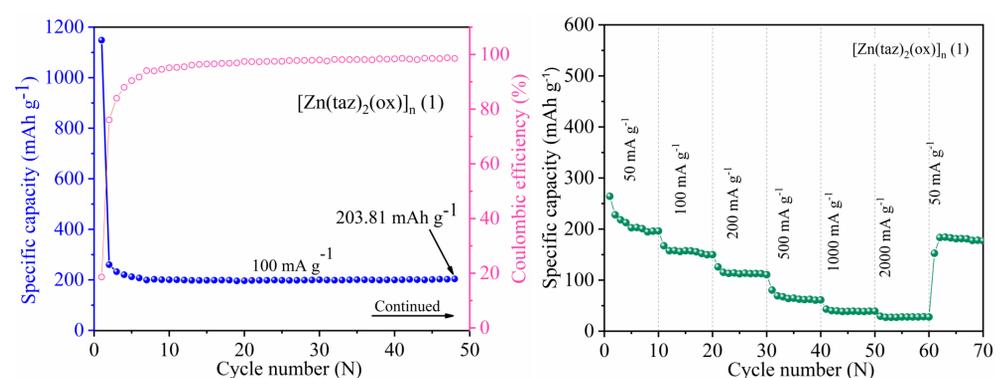


Figure 2. (a) Cycle stability and the corresponding Coulombic efficiency at a current density of 100 mA g<sup>-1</sup> for 49 cycles and (b) Rate performance at each current density.

## Acknowledgements