

## Supporting information

### Two solvent-dependent zinc(II) supramolecular isomers: Structure analysis, reversible and nonreversible crystal-to-crystal transformation, highly selective CO<sub>2</sub> gas adsorption, and photoluminescence behaviors†

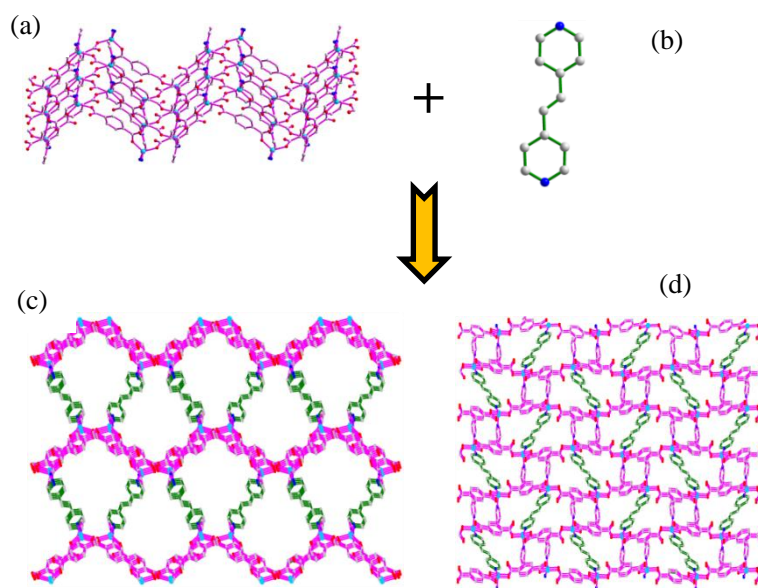
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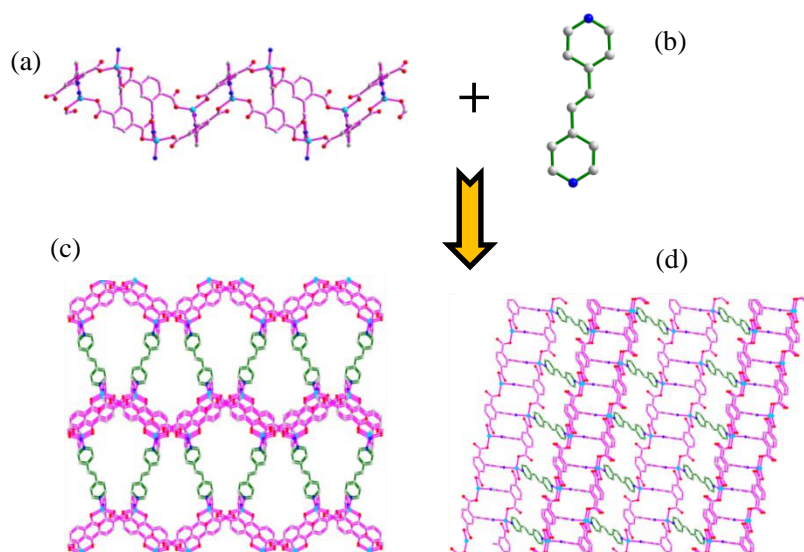
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### Table of Content

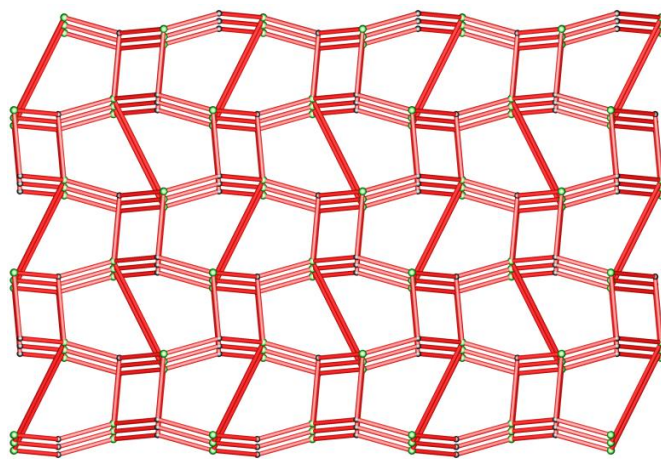
1. **Fig. S1** The 2D layer in **1** linked by Zn(II) ions and dcpy<sup>2-</sup> (a); the bpe ligand (b); view of the individual 3D structure of **1** along the *c*-axes (c) and the *a*-axes (d).
2. **Fig. S2** The 1D zigzag chain in **2** linked by Zn(II) ions and dcpy<sup>2-</sup> (a); the bpe ligand (b); view of the individual 3D structure of **1** along the *a*-axes (c) and the *c*-axes (d).
3. **Fig. S3** Ball-and-stick and schematic representations of simplified individual 3D 2-nodal (3,4)-connected topological frameworks of **1** (a) and **2** (b).
4. **Fig. S4** TGA curves for **1**, **1a**, **2**, **2a** and **2b** measured under nitrogen.
5. **Fig. S5** Variable-temperature PXRD patterns for **1** (a), and **2** (b) recorded N<sub>2</sub> atmosphere.
6. **Fig. S6** N<sub>2</sub> (77 K) and CO<sub>2</sub> (195 K) gas sorption isotherms of **2a** (the desolvated samples **2**).
7. **Fig. S7** Isothermic heat of adsorption for CO<sub>2</sub> at different CO<sub>2</sub> loadings in **1a**.



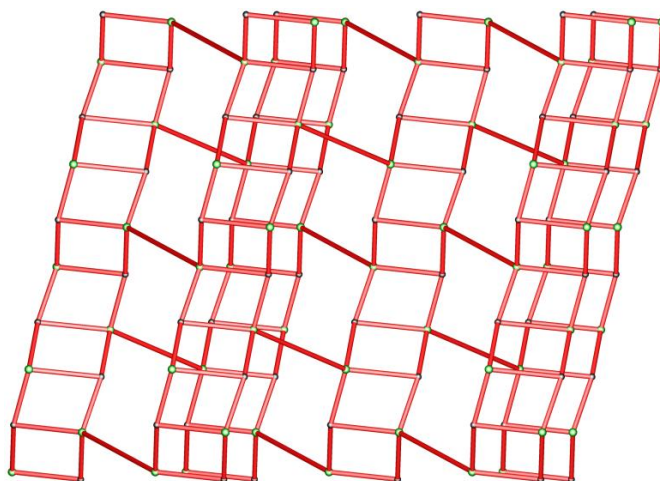
**Fig. S1** The 2D layer in **1** linked by Zn(II) ions and dcpy<sup>2-</sup> (a); the bpe ligand (b); view of the individual 3D structure of **1** along the *c*-axes (c) and the *a*-axes (d).



**Fig. S2** The 1D zigzag chain in **2** linked by Zn(II) ions and dcpy<sup>2-</sup> (a); the bpe ligand (b); view of the individual 3D structure of **1** along the *a*-axes (c) and the *c*-axes (d).

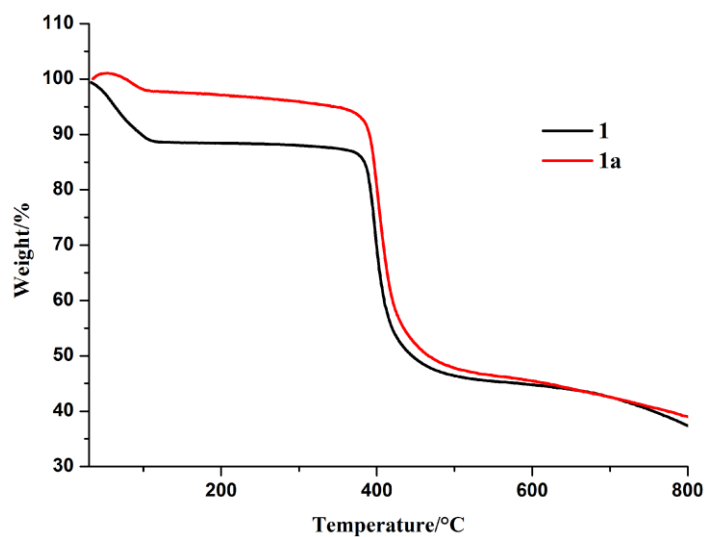


(a)

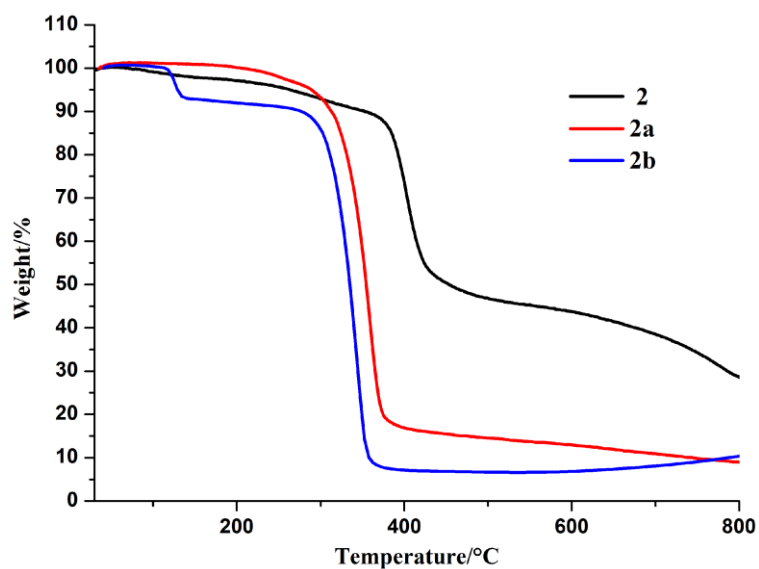


(b)

**Fig. S3** Ball-and-stick and schematic representations of simplified individual 3D 2-nodal (3,4)-connected topological frameworks of **1** (a) and **2** (b).

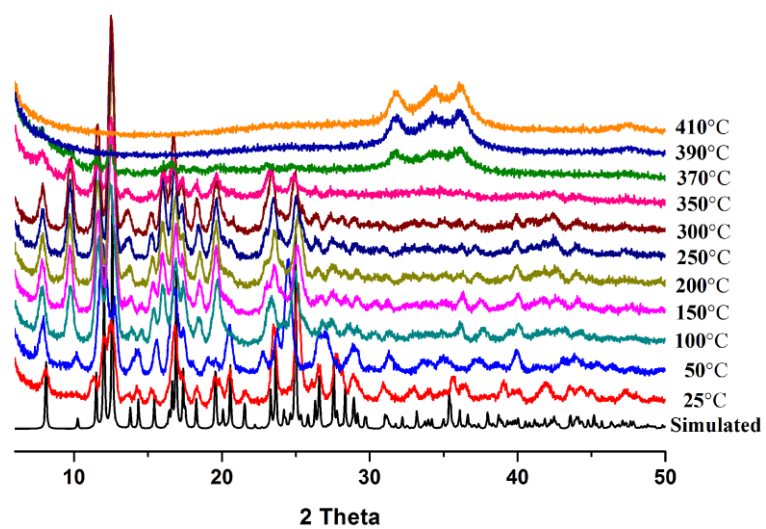


(a)

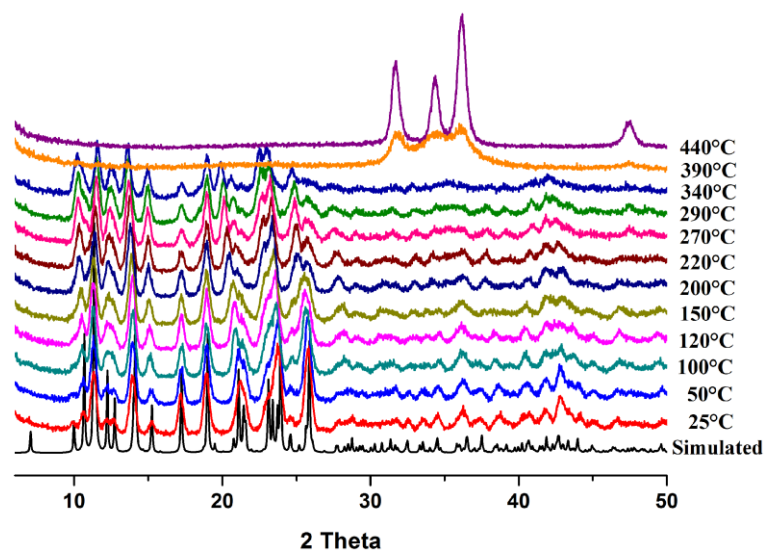


(b)

Fig. S4 TGA curves for 1, 1a, 2, 2a and 2b measured under nitrogen.

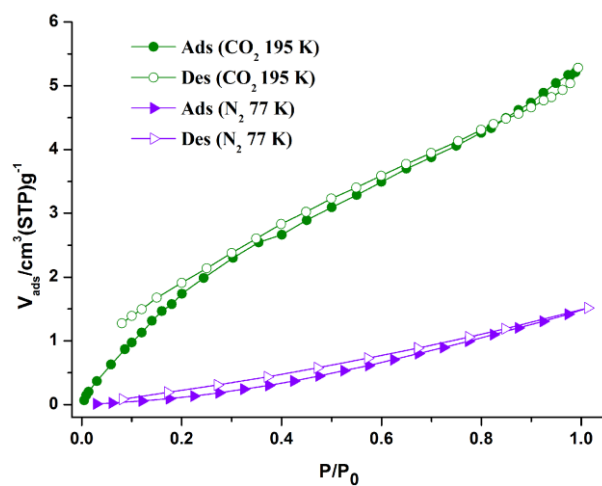


(a)

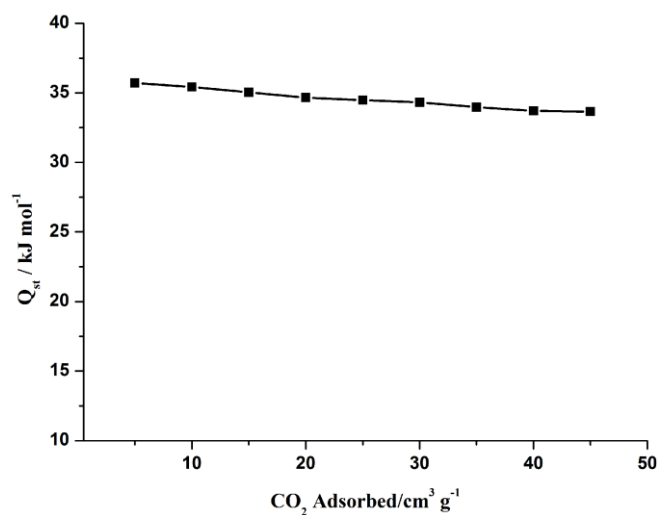


(b)

**Fig. S5** Variable-temperature PXRD patterns for **1** (a), and **2** (b) recorded N<sub>2</sub> atmosphere.



**Fig. S6** N<sub>2</sub> (77 K) and CO<sub>2</sub> (195 K) gas sorption isotherms of **2a** (the desolvated samples **2**).



**Fig. S7** Isothermic heat of adsorption for CO<sub>2</sub> at different CO<sub>2</sub> loadings in **1a**.