

Supplementary Materials for  
**Molecular-caged metal-organic frameworks for energy management**

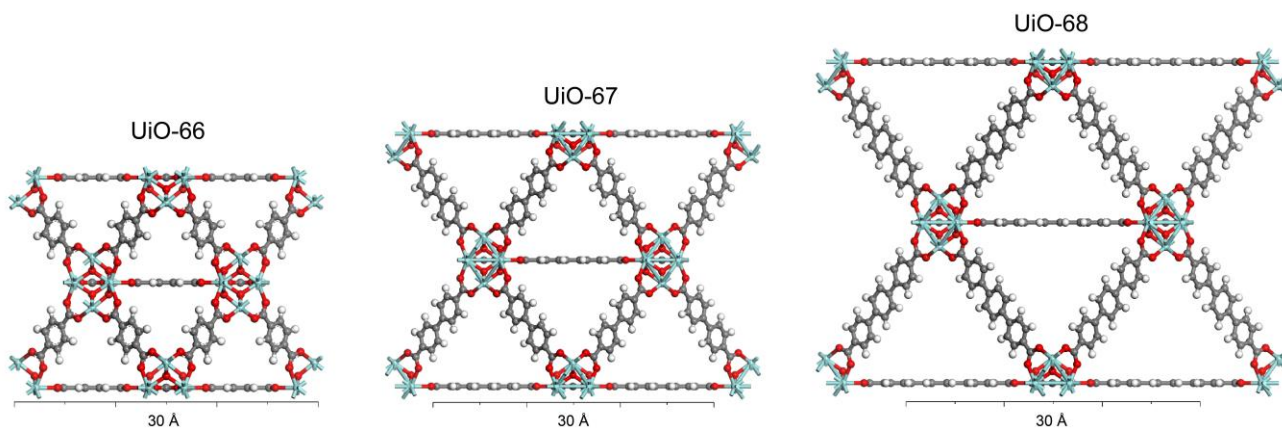
Minghong Wu *et al.*

Corresponding author: Weiqi Xie, [weiqixie@csu.edu.cn](mailto:weiqixie@csu.edu.cn); Jianqing Zhao, [psjqzhao@scut.edu.cn](mailto:psjqzhao@scut.edu.cn)

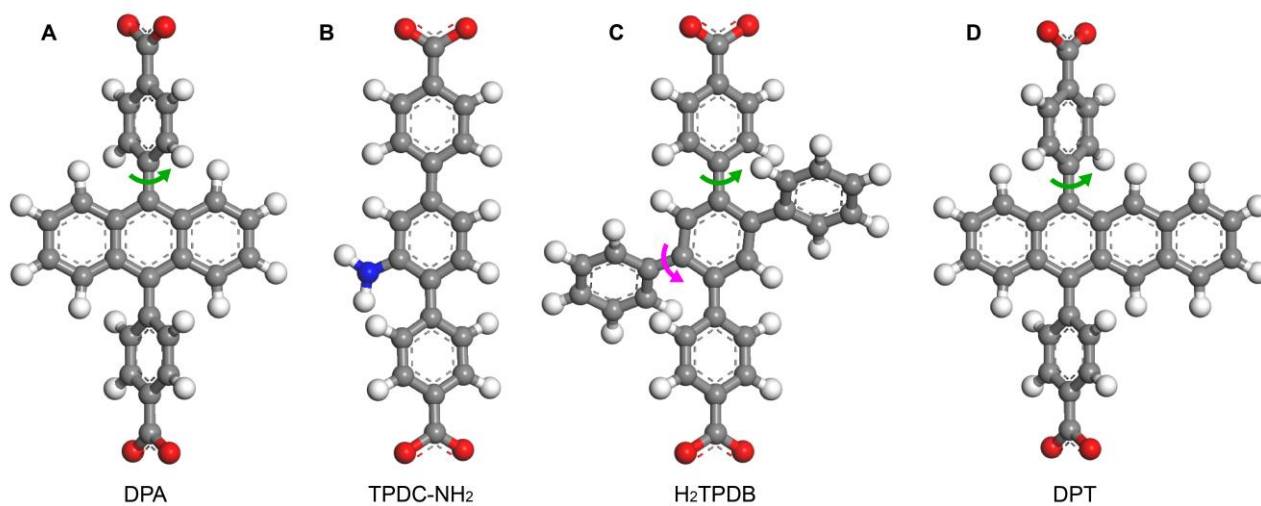
*Sci. Adv.* **10**, ead14449 (2024)  
DOI: 10.1126/sciadv.adl4449

**This PDF file includes:**

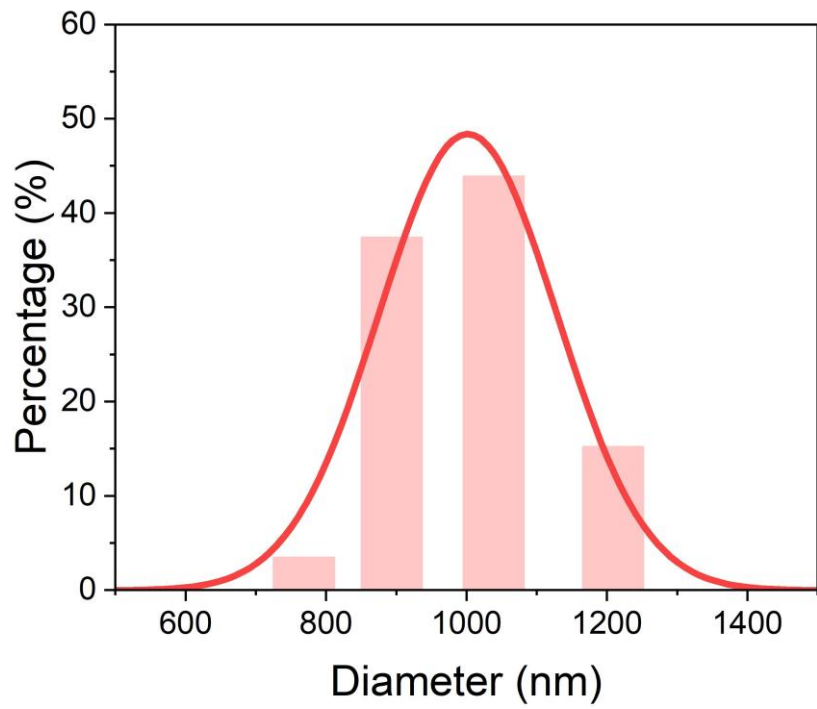
Figs. S1 to S20  
Tables S1 to S4



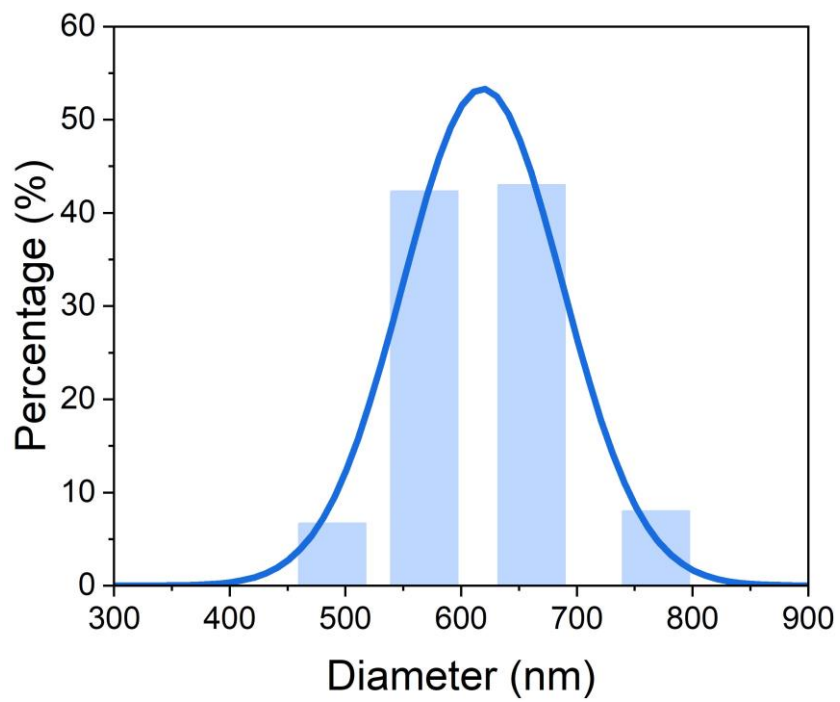
**Fig. S1** Framework structures of UiO-66, UiO-67 and UiO-68



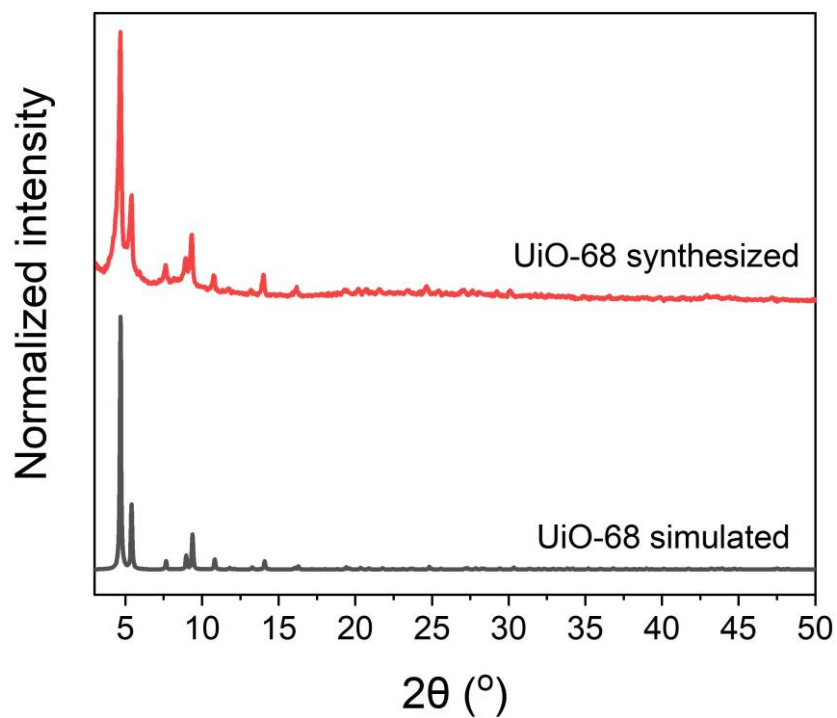
**Fig. S2** Ligand selection for constructing molecular cages



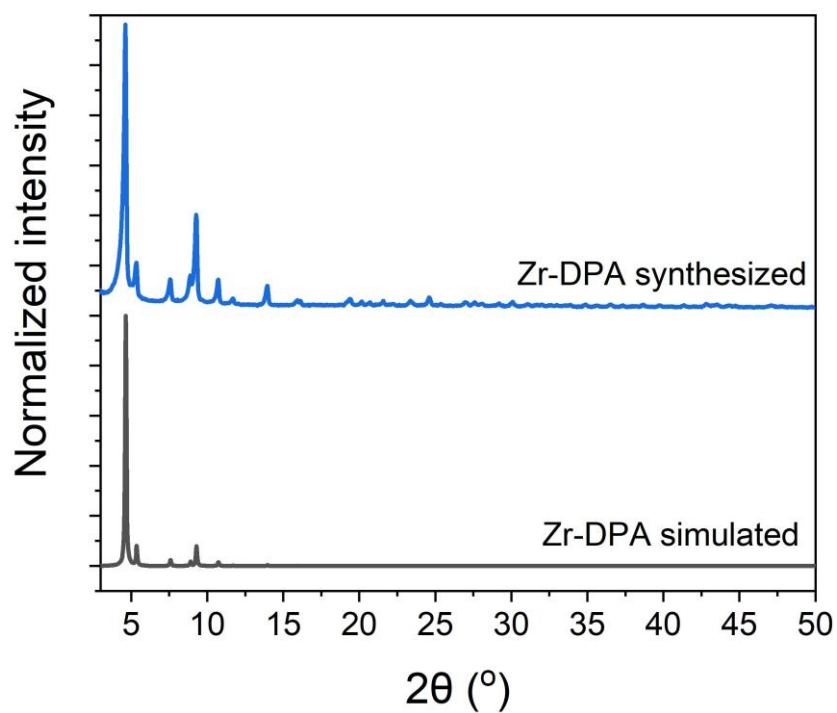
**Fig. S3** Particle size distribution of UiO-68



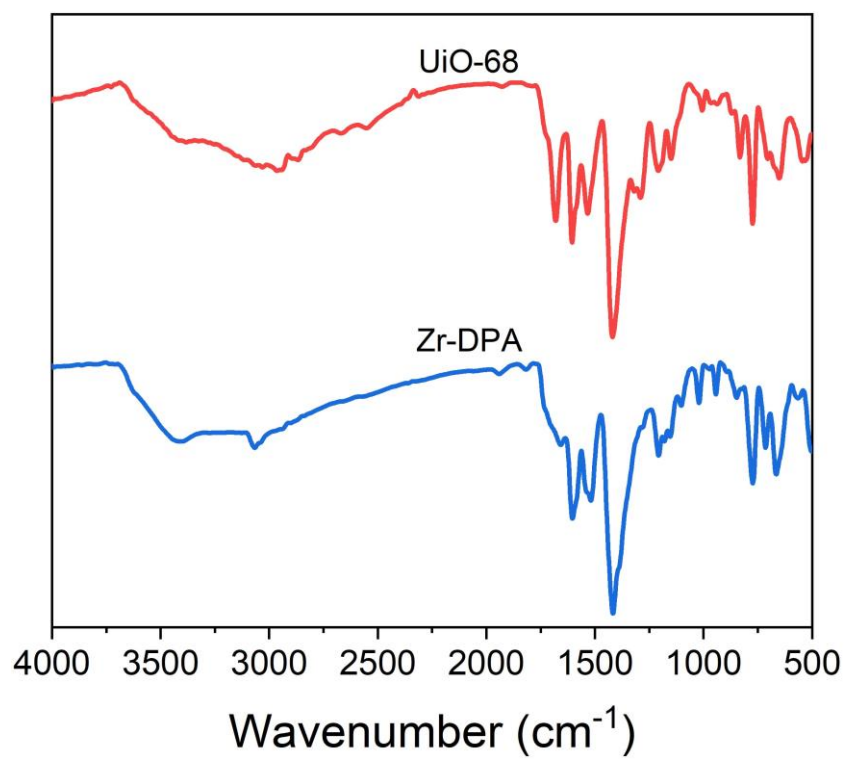
**Fig. S4** Particle size distribution of Zr-DPA



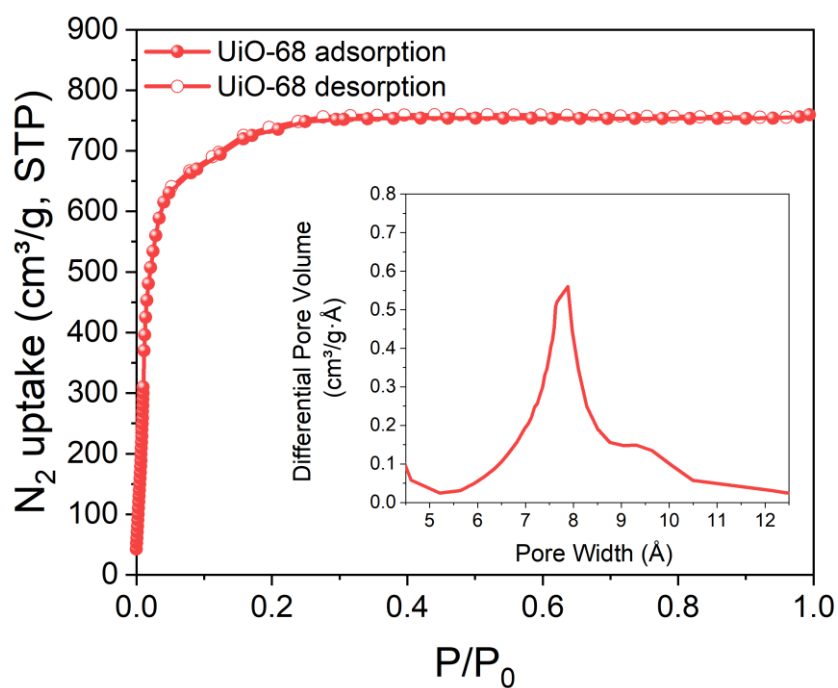
**Fig. S5** Synthesized and simulated UiO-68 XRD spectra



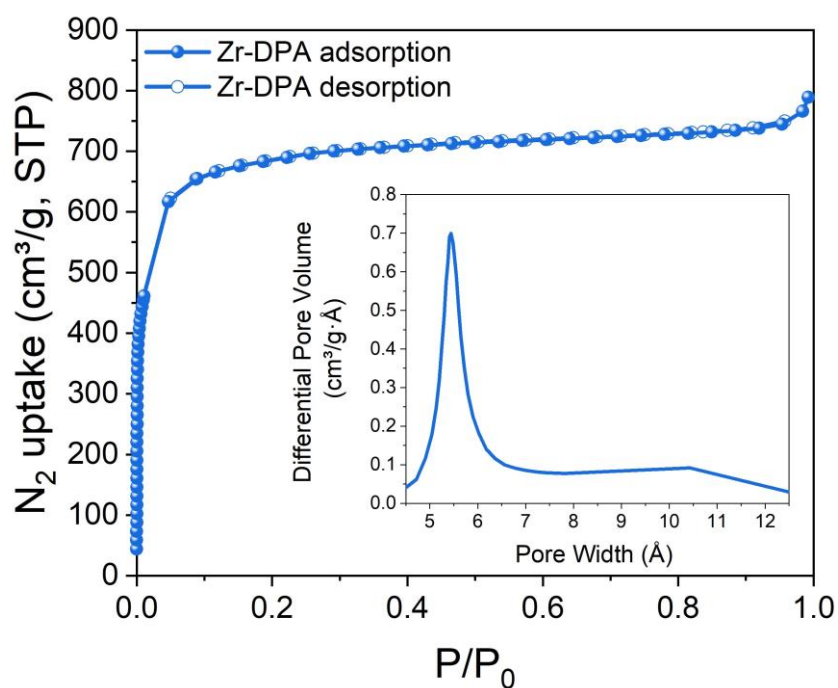
**Fig. S6** Synthesized and simulated Zr-DPA XRD spectra



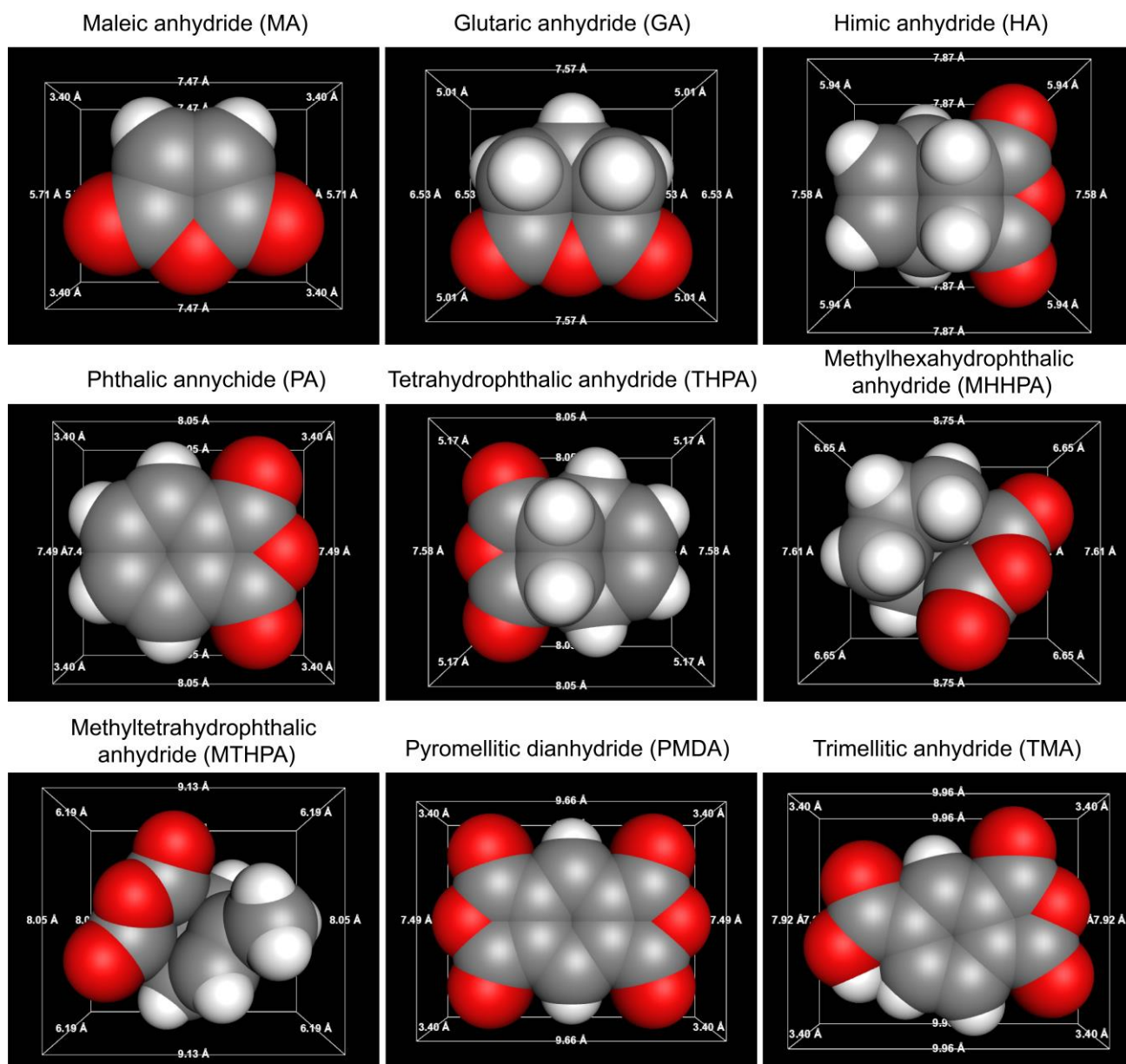
**Fig. S7** Infrared spectra of UiO-68 and Zr-DPA



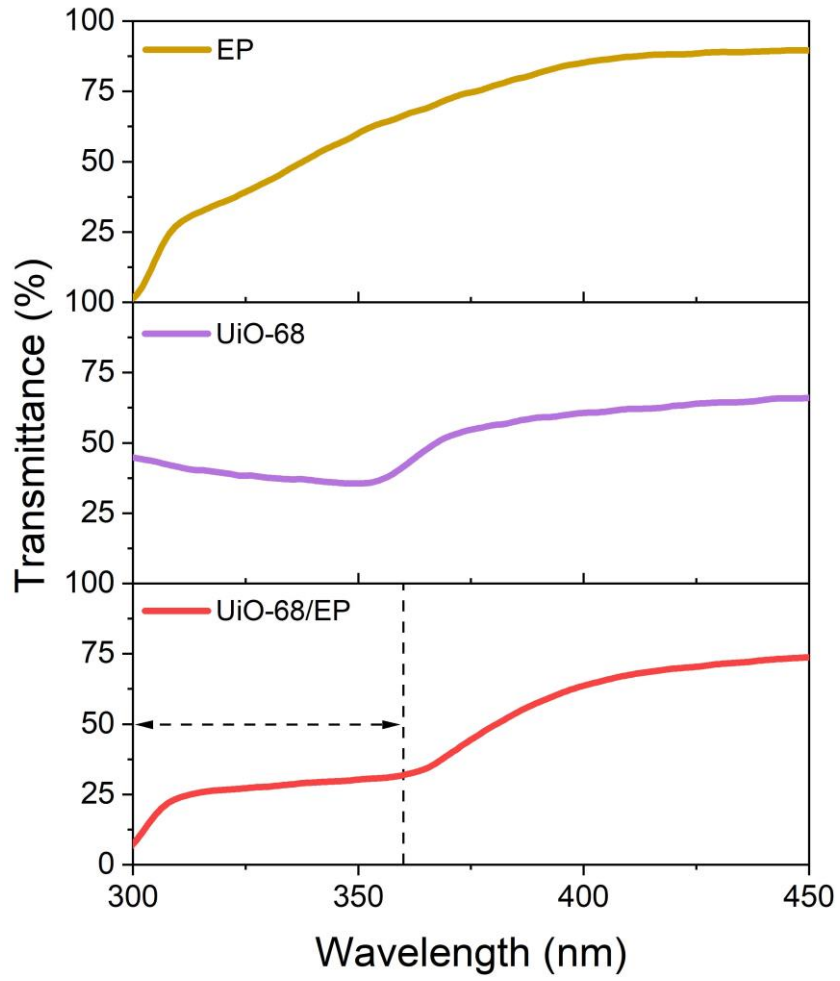
**Fig. S8** Nitrogen adsorption-desorption curves and microporous analysis of UiO-68



**Fig. S9** Nitrogen adsorption-desorption curves and microporous analysis of Zr-DPA

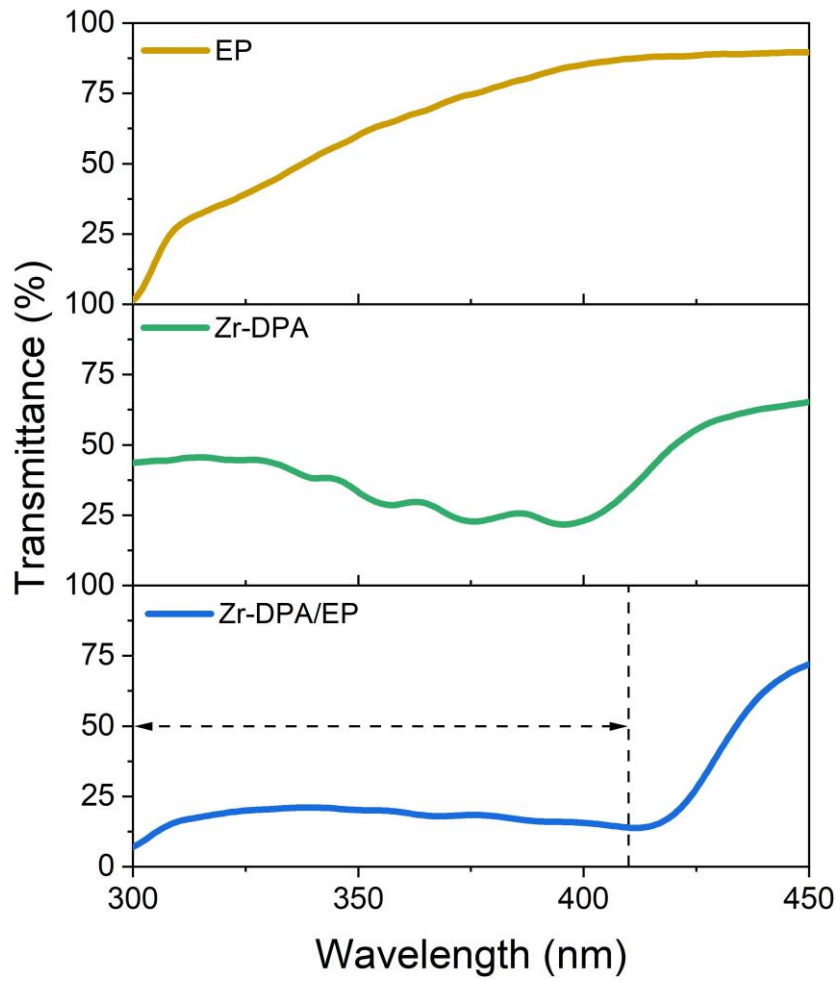


**Fig. S10** Molecular sizes of nine common epoxy anhydride curing agents

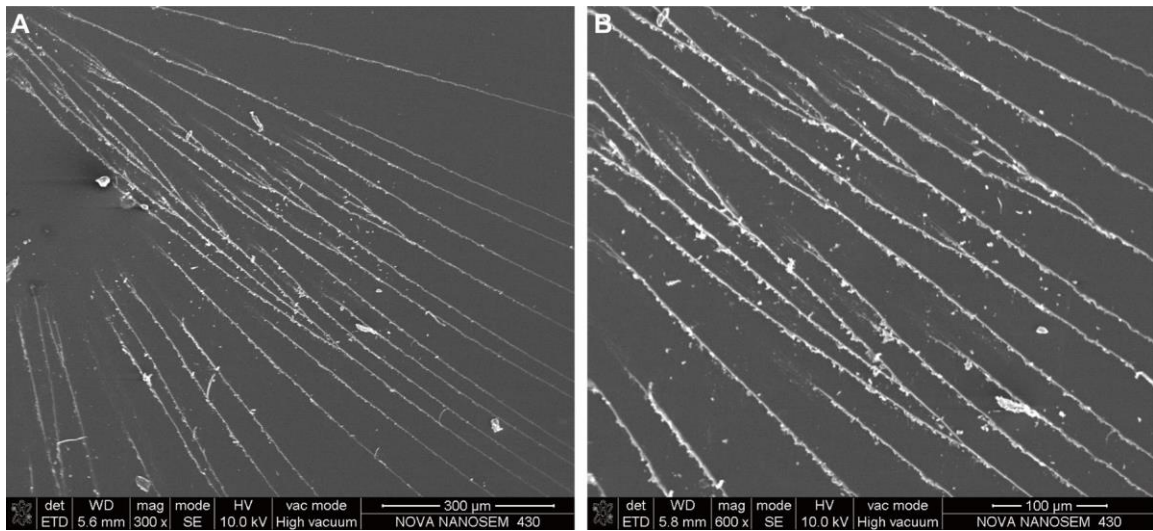


**Fig. S11** Construction process of UV shielding in UiO-68/EP

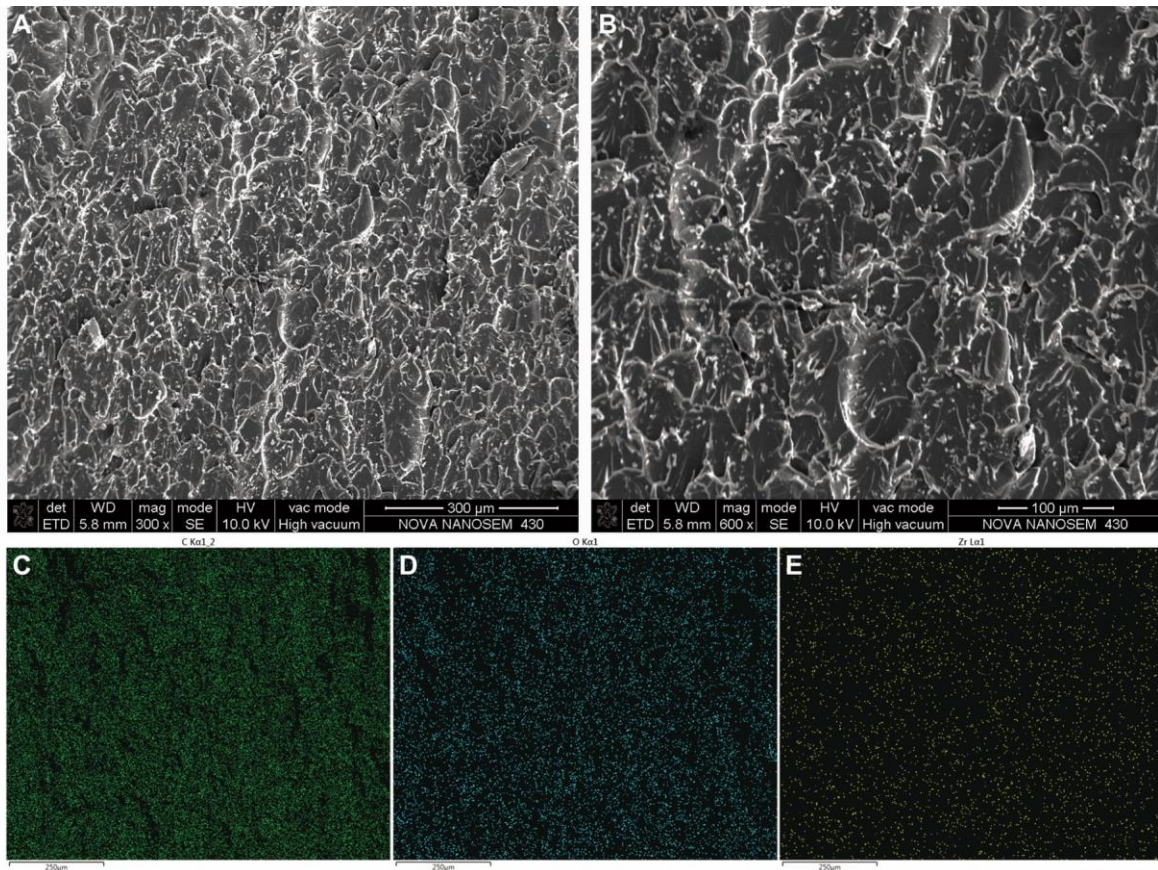




**Fig. S12** Construction process of UV shielding in Zr-DPA/EP

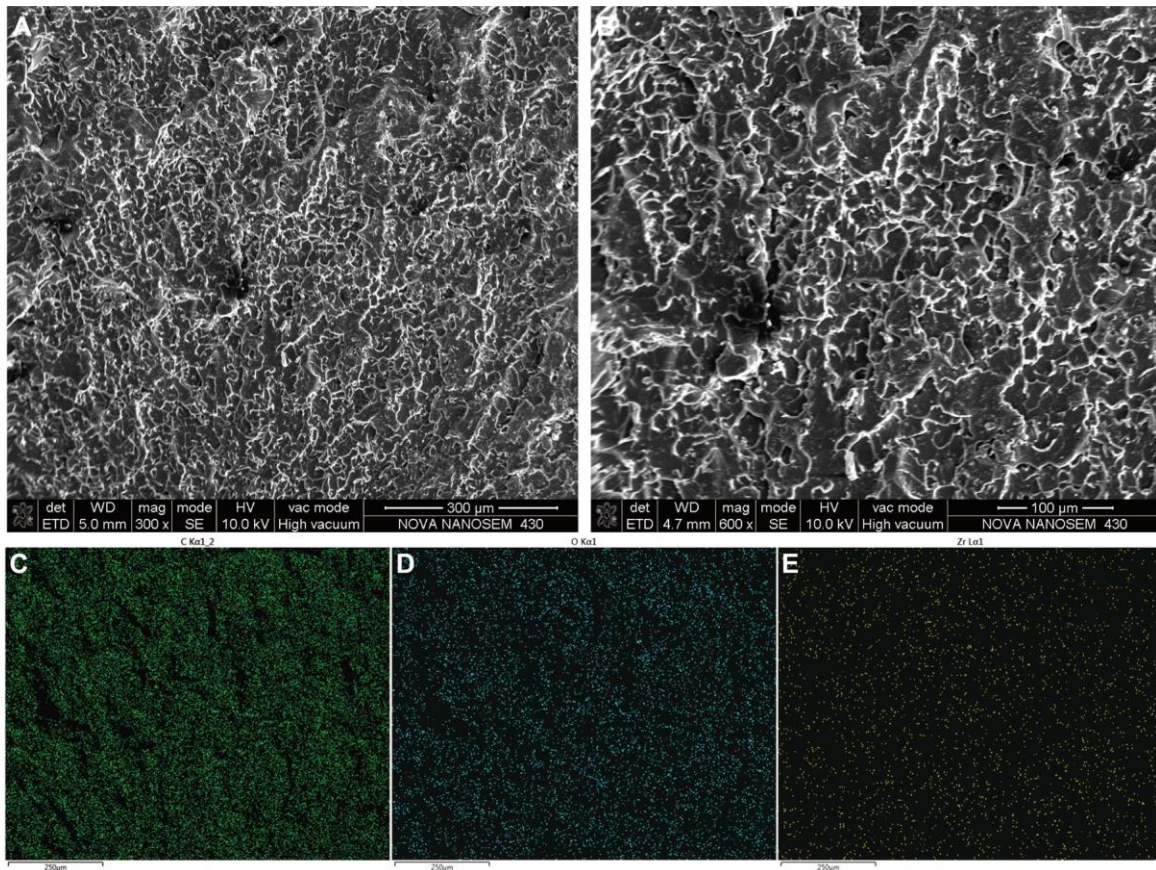


**Fig. S13** SEM micrographs of the fracture surface of pure EP at (A) 300x magnification and (B) 600x magnification.

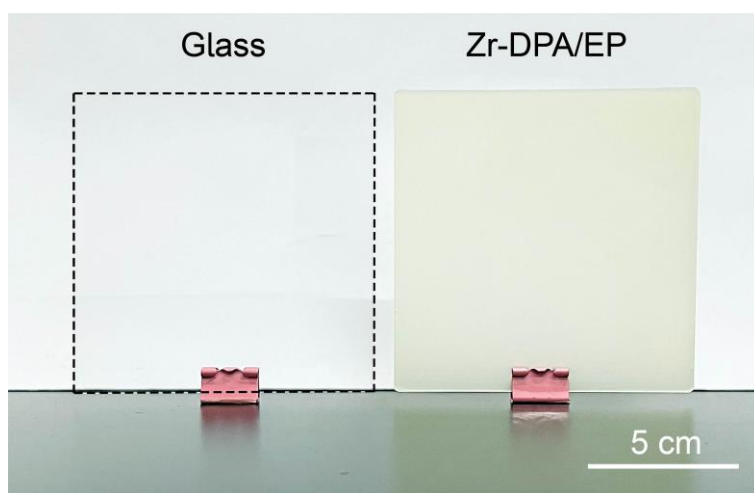


**Fig. S14** SEM micrographs of the fracture surface of UiO-68/EP at (A) 300x magnification and (B) 600x magnification. EDS mapping and elemental distributions of (C) C, (D) O and (E) Zr

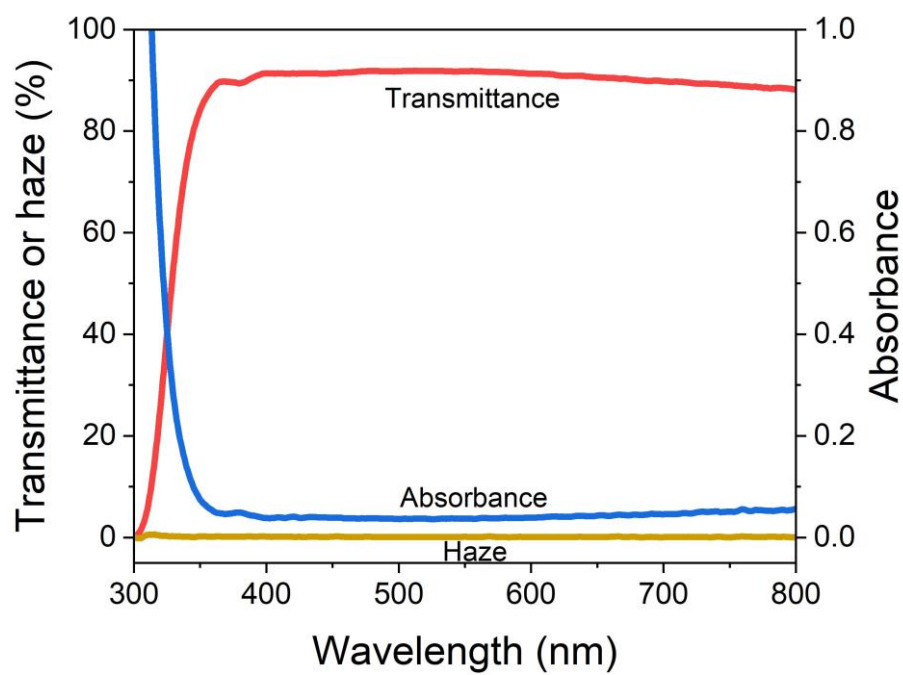




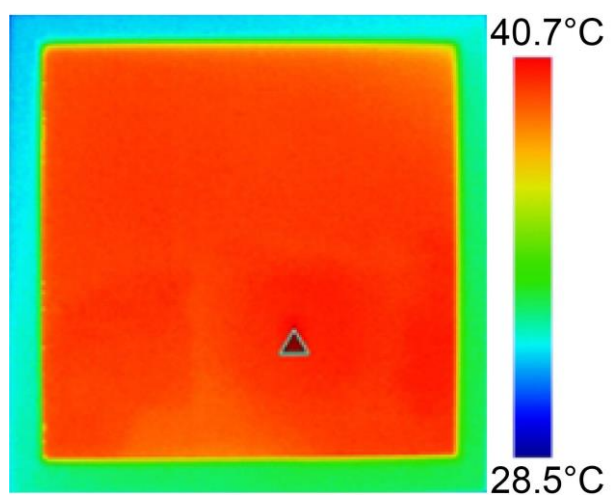
**Fig. S15** SEM micrographs of the fracture surface of Zr-DPA/EP at (A) 300x magnification and (B) 600x magnification. EDS mapping and elemental distributions of (C) C, (D) O and (E) Zr



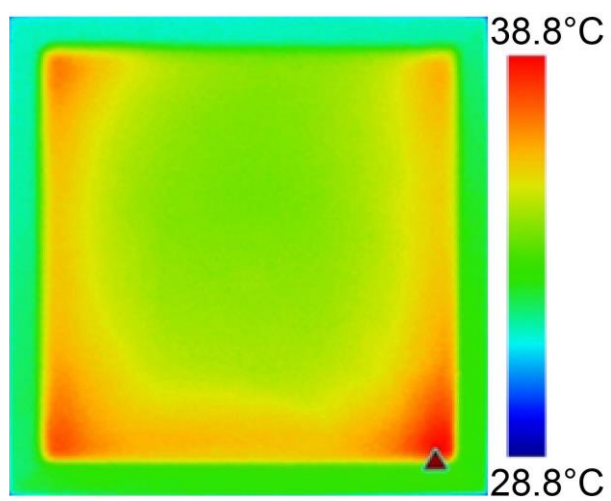
**Fig. S16** Photographs of glass and Zr-DPA/EP large samples



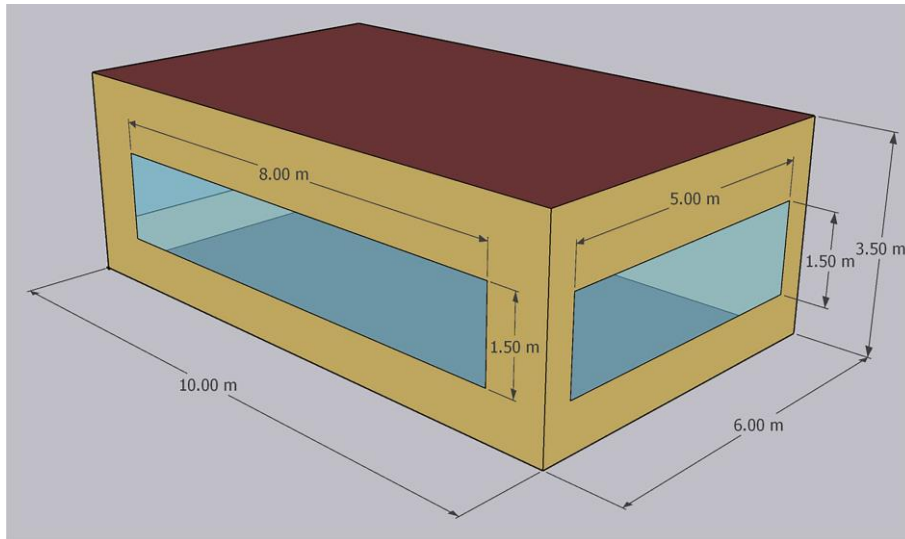
**Fig. S17** optical properties of glass



**Fig. S18** Infrared thermal imaging of glass after 30s on a hot plate



**Fig. S19** Infrared thermal imaging of Zr-DPA/EP after 30s on a hot plate



**Fig. S20** Building models for Energyplus simulation

**Table S1** Oxygen transmission rate (OTR) of the MOF/Polymer

Samples	OTR (mL m <sup>-2</sup> day <sup>-1</sup> )
Pure EP	26±4
UiO-68/EP	1600±300
Zr-DPA/EP	5700±1300



**Table S2** Comparison of this work with previously reported epoxy-containing optical composites in terms of transmittance and haze

Materials	Transmittance	Haze	Ref. (in main article)
Solar-assisted TW*	90	60	25
MTB	69	50	26
Aesthetic TW	80	93	27
Anisotropic TW	80	90	28
UFT	80	58	29
PSMTW	60	95	30
TBW	88	74	31
EP/DDM/PB-5	67	22	32
EP-DDT7	75	11	33
W/VO <sub>2</sub> -TPW-L	68	97	34
EP/4DIT	89	14	35
TB** with PTGE	79	72	36
Zr-DPA/EP	83	93	This work

TW\* represents transparent wood filled with epoxy resin.

TB\*\* represents transparent bamboo filled with epoxy resin.

**Table S3** Comparison of this work with previously reported epoxy-containing composites for building in terms of thermal conductivity

Materials	Thermal conductivity ( $\text{W m}^{-1} \text{K}^{-1}$ )	Ref. (in main article)
TB** with PTGE	0.35	36
Clear wood	0.35	37
TB with E51/DETA	0.33	38
ESMTW*	0.29	39
TB with Ag-80/DDM	0.25	40
Aesthetic TW	0.24	27
Silica xerogel/epoxy	0.22	41
W/VO <sub>2</sub> -TPW-L	0.20	34
TBW	0.20	31
Zr-DPA/EP	0.16	This work

TW\* represents transparent wood filled with epoxy resin.

TB\*\* represents transparent bamboo filled with epoxy resin.

**Table S4** Parameters of Zr-DPA/EP for EnergyPlus calculations

Variables	Zr-DPA/EP
Solar Transmittance	0.76
Solar Front Reflectance	0.08
Solar Back Reflectance	0.08
Visible Transmittance	0.83
Visible Front Reflectance	0.09
Visible Back Reflectance	0.09
Emissivity	0.85