Electronic Supplementary Information (ESI)

An anionic metal-organic framework with ternary building units for rapid and selective adsorption of dyes

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S1 Supporting Figures

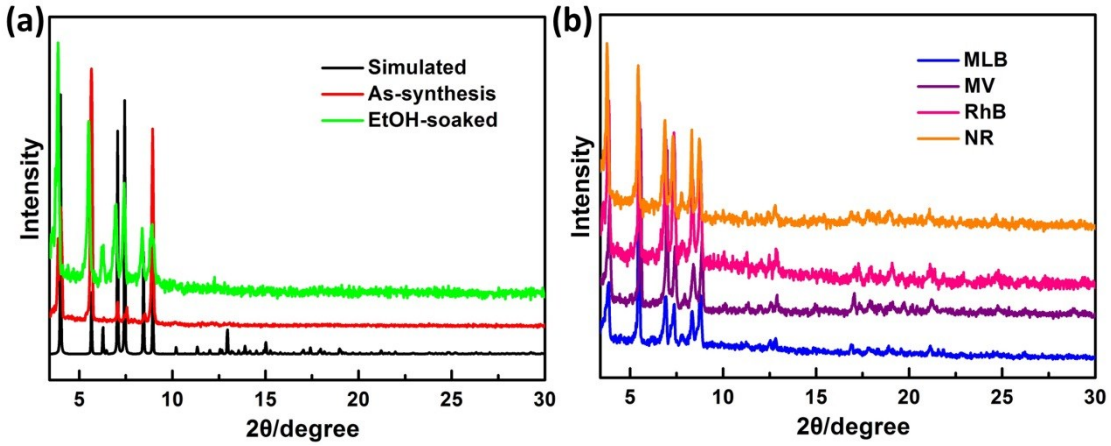


Fig. S1 (a) The PXRD patterns of simulated, as-synthesized and EtOH-soaked **JLU-Liu39**. (b) The PXRD patterns of **JLU-Liu39** after the organic dyes adsorption.

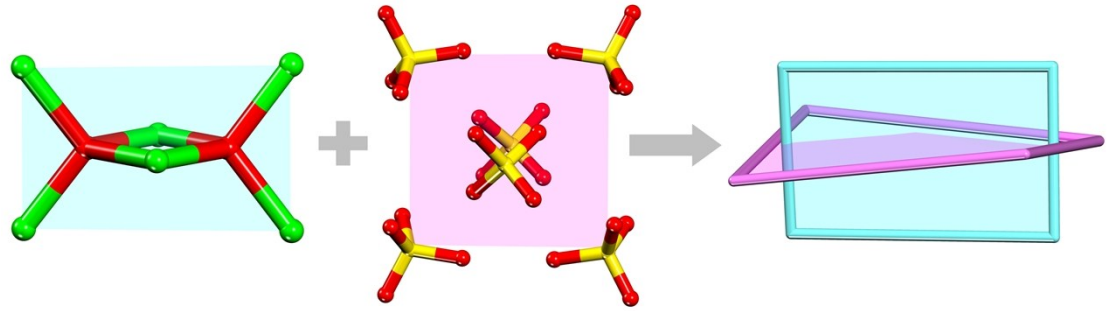


Fig. S2 The relative position of the six coppers and six sulphate radicals in the hexa-nuclear $[Cu_6O_2(SO_4)_6L_4]$ cluster.

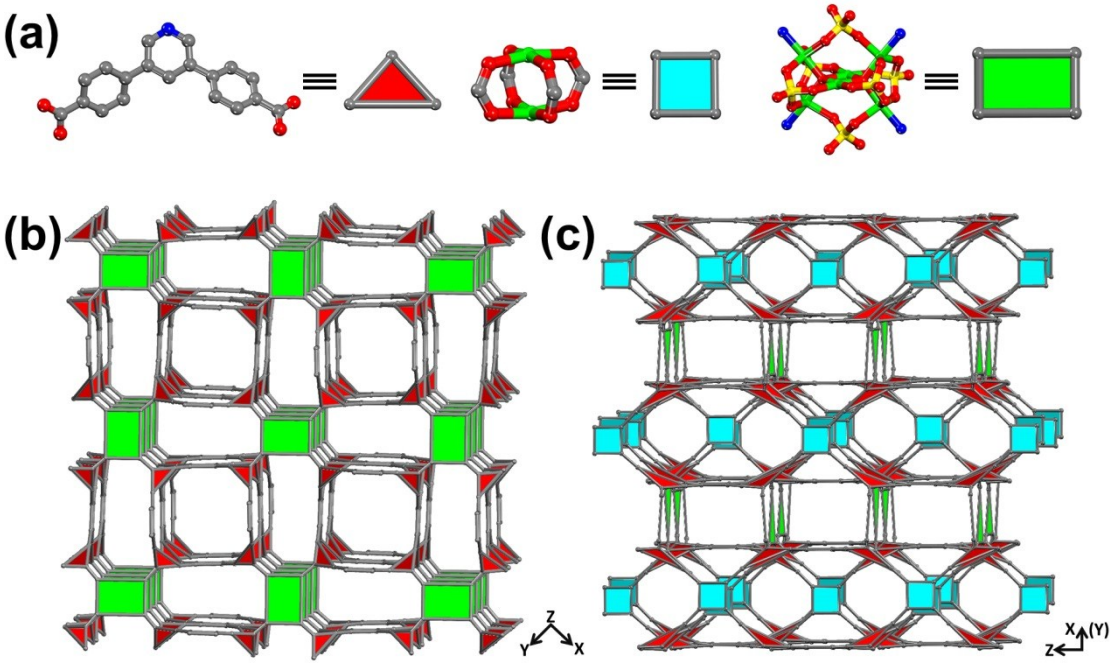


Fig. S3 Polyhedral views of **JLU-Liu39** along the directions of [001] and [110].

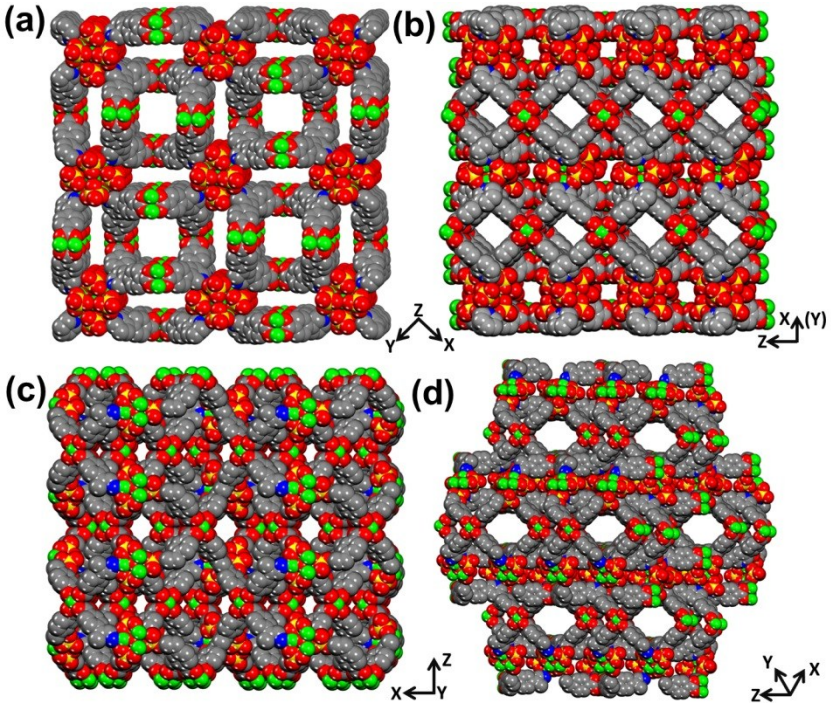


Fig. S4 Space-filling models of **JLU-Liu39** along different directions.

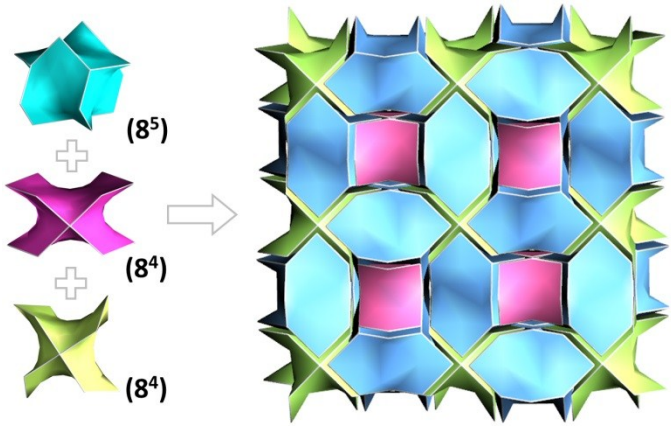


Fig. S5 Topological features of **JLU-Liu39** displayed by tiles and face symbols for blue, pink and yellow tiles are (8^5), (8^4) and (8^4).

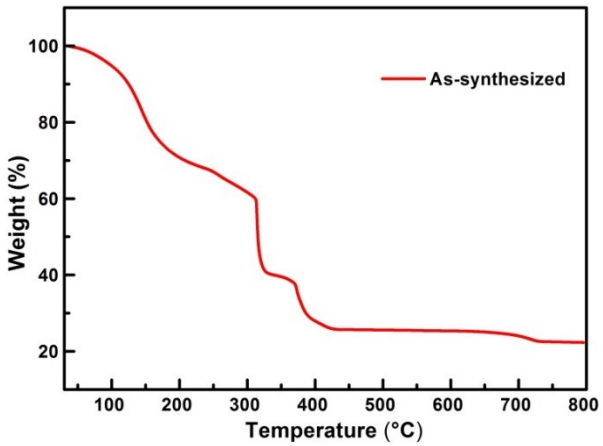


Fig. S6 TGA curve for the as-synthesized **JLU-Liu39**.

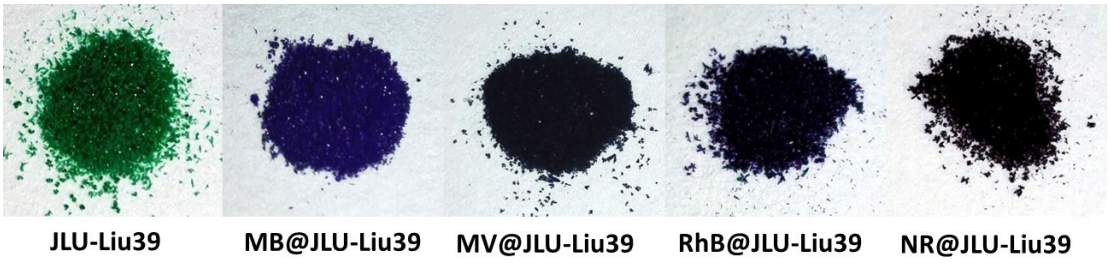


Fig. S7 Photographs of the dyes adsorbed crystals of **JLU-Liu39**.

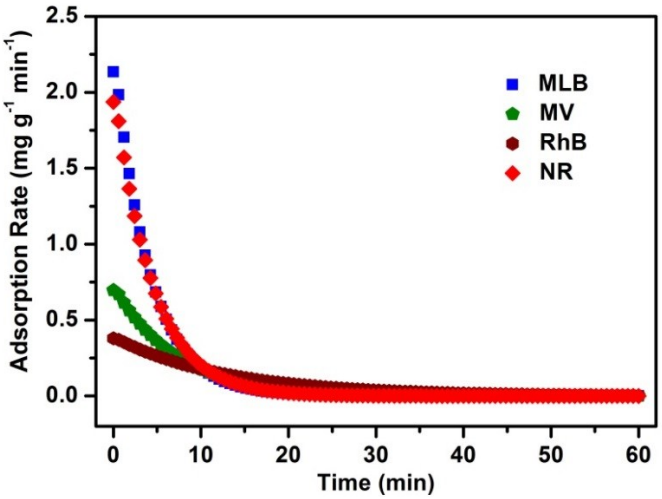


Fig. S8 The first-order derivative curves of adsorption amount (Qe) with time for MLB, MV, RhB and NR.

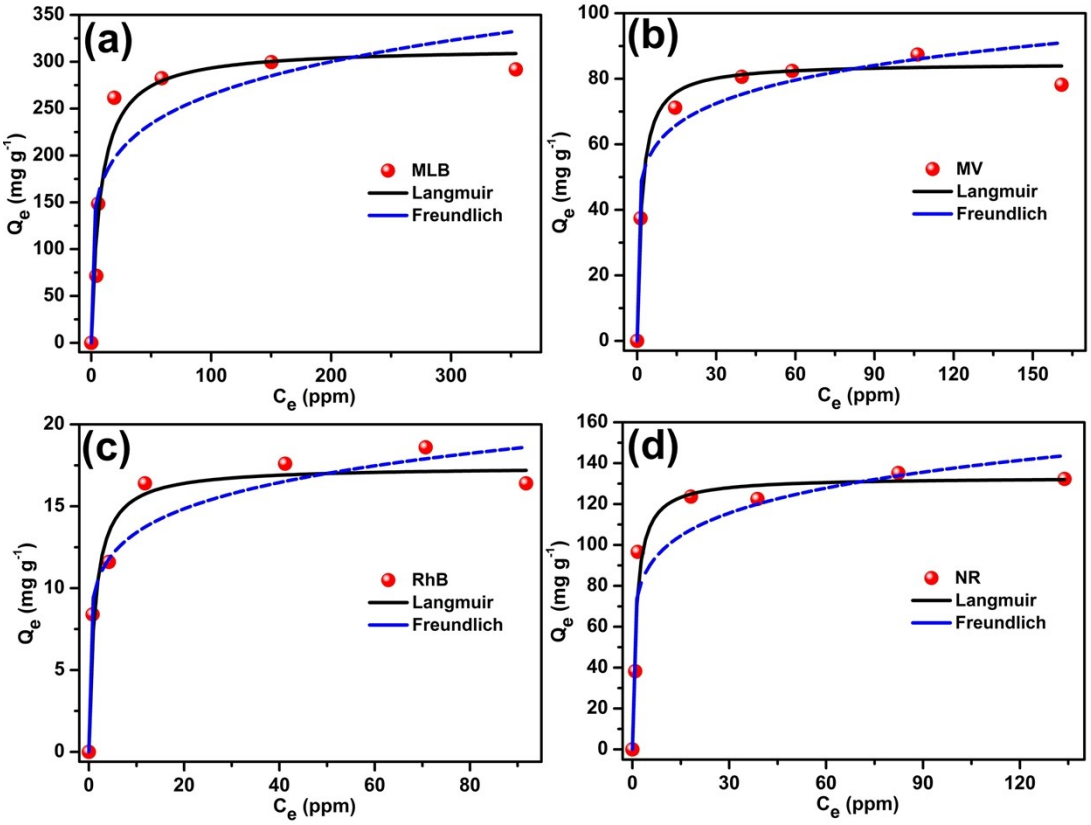


Fig. S9 Langmuir and Freundlich isotherms fitting plots for the adsorption of MLB (a), MV (b), RhB (c) and NR (d).

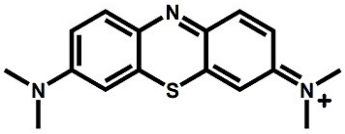
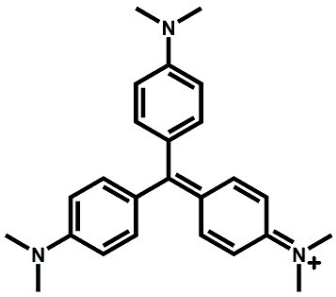
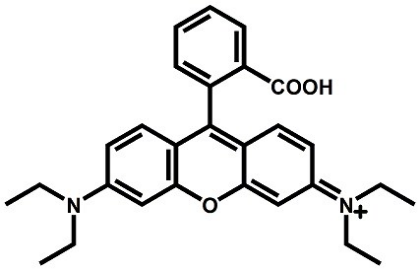
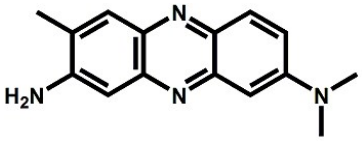
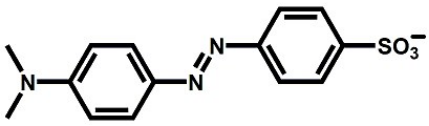
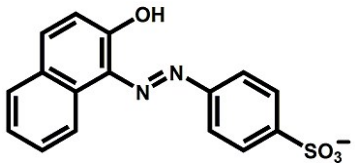
Table S1 Crystal data and structure refinements for JLU-Liu39

Compound	**JLU-Liu39**
Formula	$C_{72}\ H_{110}\ Cu_5\ N_{14}\ O_{32}\ S_3$
Mw	2097.61
Temperature (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	Tetragonal
Space group	$P4_2/mbc$
a (Å)	31.236(4)
b (Å)	31.236(4)
c (Å)	28.194(5)
V (Å^3)	27509(9)
Z, D_c (Mg/m^3)	8, 1.013
F(000)	8712
θ range (deg)	0.922 -25.162
Reflns collected/unique	175094/12562
R_{int}	0.1560
data/restraints/params	12562/0/328
GOF on F^2	0.983
R_1, wR_2 (I>2σ(I))	0.0616, 0.1989
R_1, wR_2 (all data)	0.1432, 0.2956

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR_2 = [\Sigma w(|F_o|^2 - |F_c|^2)/\Sigma|w(F_o^2)^2|]^{1/2}$

PLATON/SQUEEZE was employed to calculate the diffraction contribution of the solvent molecules and, thereby, to produce a set of solvent-free diffraction intensities; structures were then refined again using the generated data. Since the highly disordered cations and guest molecules were trapped in the channels of **JLU-Liu39** and could not be modeled properly, there are "Alert level A" in the "checkCIF/PLATON report" files for **JLU-Liu39**. The final formulas of **JLU-Liu39** were derived from crystallographic data combined with elemental and thermogravimetric analysis data.

Table S2 Dimensions of dye molecules with different charges.

Dye name	Chemical structures	Ionicity	Dimensions (nm)
Methylene Blue (MLB)		Cationic	1.38×0.64×0.21
Methyl Violet (MV)		Cationic	1.42×1.01×0.22
Rhodamine B (RhB)		Cationic	1.56×1.35×0.42
Neutral Red (NR)		Neutral	1.26×0.64×0.23
Methyl Orange (MO)		Anionic	1.54×0.48×0.28
Orange II		Anionic	1.35×0.72×0.28