Supplementary Information

A new {Cu_3-Gd_2} cluster as two-in-one functional material with unique topology acting as a refrigerant as well as adsorbent for cationic dye

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Table S1. Crystal structure refinement data for **{Cu_3-Gd_2}.**

CCDC No.	2141839
Empirical formula	$C_{34}H_{70}Cu_3Gd_2N_4O_{27}$
Formula weight	1472.09
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.9919(4)
b/Å	18.7337(6)
c/Å	13.0670(4)
α/°	90
β/°	108.8720(10)
γ/°	90
Volume/Å^3	2777.73(15)
Z	2
ρ_{calc}g/cm^3	1.7599
μ/mm^{-1}	3.566
F(000)	1469.2
Crystal size/mm^3	0.33 × 0.23 × 0.16
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.6 to 50.1
Index ranges	$-15 \le h \le 15$, $-24 \le k \le 24$, $-17 \le l \le 17$
Reflections collected	43485
Independent reflections	4918 [R_{int} = 0.0593, R_{sigma} = 0.0376]
Data/restraints/parameters	4918/0/343
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0246, wR_2 = 0.0591
Final R indexes [all data]	R_1 = 0.0306, wR_2 = 0.0633
Largest diff. peak/hole / e Å^{-3}	0.62/-0.61

Table S2. Selected bond lengths (Å) for **{Cu_3-Gd_2}.**

Atom Atom		Length/Å	Atom Atom		Length/Å
Gd1	Cu1	3.3037(5)	O3	C4	1.417(5)
Gd1	Cu2	3.41601(19)	O4	C10	1.409(4)
Gd1	O1	2.288(2)	O5	C11	1.429(4)
Gd1	O4[1]	2.363(2)	O6	C9	1.416(5)
Gd1	O5	2.423(2)	O7	C12	1.261(5)
Gd1	O7	2.518(3)	O8	C12	1.262(5)
Gd1	O8	2.478(3)	O9	C14	1.259(5)
Gd1	O9	2.631(3)	O10	C14	1.269(5)
Gd1	O10	2.446(3)	O11	C16	1.267(5)
Gd1	O11	2.480(3)	O12	C16	1.266(5)
Gd1	O12	2.425(3)	N1	C2	1.503(5)
Gd1	C12	2.879(4)	N1	C5	1.483(5)
Gd1	C14	2.915(4)	N2	C7	1.491(5)
Gd1	C16	2.825(4)	N2	C8	1.506(4)
Cu1	Cu2[1]	2.8610(4)	C1	C2	1.535(5)
Cu1	O1	1.910(3)	C2	C3	1.532(5)
Cu1	O2	2.440(3)	C2	C4	1.525(5)
Cu1	O5	1.975(2)	C5	C6	1.514(5)
Cu1	N1	1.982(3)	C6	C7	1.535(5)
Cu1	N2	1.974(3)	C8	C9	1.527(5)
Cu2	O4[1]	1.915(2)	C8	C10	1.525(5)
Cu2	O4	1.915(2)	C8	C11	1.521(5)
Cu2	O5	1.976(2)	C12	C13	1.496(5)
Cu2	O5[1]	1.976(2)	C14	C15	1.503(6)
O1	C1	1.410(4)	C16	C17	1.493(6)
O2	C3	1.434(4)			

Table S3. Selected bond angles for **{Cu_3-Gd_2}.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cu2	Gd1	Cu1	50.364(8)	N1	Cu1	Cu2[1]	133.11(9)
O1	Gd1	Cu1	34.22(6)	N1	Cu1	O1	87.27(12)
O1	Gd1	Cu2	68.28(6)	N1	Cu1	O2	74.67(11)
O4[1]	Gd1	Cu1	78.19(6)	N1	Cu1	O5	173.75(12)
O4[1]	Gd1	Cu2	32.70(6)	N2	Cu1	Gd1	128.08(9)
O4[1]	Gd1	O1	81.30(9)	N2	Cu1	Cu2[1]	96.47(9)
O5	Gd1	Cu1	36.41(6)	N2	Cu1	O1	167.52(12)
O5	Gd1	Cu2	34.54(6)	N2	Cu1	O2	111.93(11)
O5	Gd1	O1	69.22(8)	N2	Cu1	O5	86.49(11)
O5	Gd1	O4[1]	66.74(8)	N2	Cu1	N1	99.52(13)
O7	Gd1	Cu1	62.08(6)	Gd1[1]	Cu2	Gd1	180.0
O7	Gd1	Cu2	105.50(6)	Cu1[1]	Cu2	Gd1[1]	62.782(9)
O7	Gd1	O1	73.73(9)	Cu1	Cu2	Gd1	62.782(9)
O7	Gd1	O4[1]	137.92(9)	Cu1[1]	Cu2	Gd1	117.218(9)
O7	Gd1	O5	72.87(8)	Cu1	Cu2	Gd1[1]	117.218(9)
O8	Gd1	Cu1	106.39(6)	Cu1[1]	Cu2	Cu1	180.0
O8	Gd1	Cu2	122.19(7)	O4[1]	Cu2	Gd1[1]	138.19(7)
O8	Gd1	O1	125.55(9)	O4	Cu2	Gd1	138.19(7)
O8	Gd1	O4[1]	139.03(9)	O4	Cu2	Gd1[1]	41.81(7)
O8	Gd1	O5	92.55(9)	O4[1]	Cu2	Gd1	41.81(7)
O8	Gd1	O7	51.81(9)	O4[1]	Cu2	Cu1[1]	82.40(7)
O9	Gd1	Cu1	116.75(6)	O4	Cu2	Cu1	82.40(7)
O9	Gd1	Cu2	77.52(6)	O4[1]	Cu2	Cu1	97.60(7)
O9	Gd1	O1	145.55(9)	O4	Cu2	Cu1[1]	97.60(7)
O9	Gd1	O4[1]	71.76(8)	O4[1]	Cu2	O4	180.0
O9	Gd1	O5	80.43(8)	O5[1]	Cu2	Gd1[1]	44.06(7)
O9	Gd1	O7	113.09(9)	O5	Cu2	Gd1	44.06(7)
O9	Gd1	O8	70.08(9)	O5	Cu2	Gd1[1]	135.94(7)
O10	Gd1	Cu1	164.36(6)	O5[1]	Cu2	Gd1	135.94(7)
O10	Gd1	Cu2	114.09(6)	O5	Cu2	Cu1[1]	136.41(7)
O10	Gd1	O1	150.22(9)	O5[1]	Cu2	Cu1	136.41(7)
O10	Gd1	O4[1]	87.74(8)	O5[1]	Cu2	Cu1[1]	43.59(7)
O10	Gd1	O5	130.77(8)	O5	Cu2	Cu1	43.59(7)
O10	Gd1	O7	129.17(9)	O5[1]	Cu2	O4[1]	94.83(10)
O10	Gd1	O8	79.84(9)	O5[1]	Cu2	O4	85.17(10)
O10	Gd1	O9	51.09(9)	O5	Cu2	O4[1]	85.17(10)
O11	Gd1	Cu1	110.74(6)	O5	Cu2	O4	94.83(10)
O11	Gd1	Cu2	109.07(6)	O5[1]	Cu2	O5	180.0

O11	Gd1	O1	77.35(9)	Cu1	O1	Gd1	103.44(10)
O11	Gd1	O4[1]	83.79(8)	C1	O1	Gd1	144.4(2)
O11	Gd1	O5	137.84(8)	C1	O1	Cu1	110.8(2)
O11	Gd1	O7	121.62(9)	C3	O2	Cu1	103.7(2)
O11	Gd1	O8	128.37(9)	Cu2[1]	O4	Gd1[1]	105.49(10)
O11	Gd1	O9	119.31(9)	C10	O4	Gd1[1]	119.5(2)
O11	Gd1	O10	73.97(9)	C10	O4	Cu2[1]	121.7(2)
O12	Gd1	Cu1	111.64(7)	Cu1	O5	Gd1	96.84(9)
O12	Gd1	Cu2	152.38(6)	Cu2	O5	Gd1	101.40(10)
O12	Gd1	O1	85.95(9)	Cu2	O5	Cu1	92.80(10)
O12	Gd1	O4[1]	136.84(9)	C11	O5	Gd1	132.2(2)
O12	Gd1	O5	143.71(9)	C11	O5	Cu1	107.1(2)
O12	Gd1	O7	75.04(9)	C11	O5	Cu2	117.6(2)
O12	Gd1	O8	80.52(9)	C12	O7	Gd1	93.2(2)
O12	Gd1	O9	128.45(9)	C12	O8	Gd1	95.1(2)
O12	Gd1	O10	83.31(9)	C14	O9	Gd1	89.9(2)
O12	Gd1	O11	53.15(9)	C14	O10	Gd1	98.4(2)
C12	Gd1	Cu1	83.92(8)	C16	O11	Gd1	92.1(2)
C12	Gd1	Cu2	116.11(8)	C16	O12	Gd1	94.6(2)
C12	Gd1	O1	99.66(10)	C2	N1	Cu1	102.0(2)
C12	Gd1	O4[1]	146.01(10)	C5	N1	Cu1	117.7(2)
C12	Gd1	O5	81.72(10)	C5	N1	C2	116.6(3)
C12	Gd1	O7	25.93(10)	C7	N2	Cu1	114.7(2)
C12	Gd1	O8	25.89(10)	C8	N2	Cu1	108.7(2)
C12	Gd1	O9	91.45(10)	C8	N2	C7	116.2(3)
C12	Gd1	O10	104.73(10)	C2	C1	O1	109.8(3)
C12	Gd1	O11	129.84(10)	C1	C2	N1	105.0(3)
C12	Gd1	O12	76.72(10)	C3	C2	N1	108.7(3)
C14	Gd1	Cu1	141.46(8)	C3	C2	C1	110.7(3)
C14	Gd1	Cu2	95.85(8)	C4	C2	N1	112.0(3)
C14	Gd1	O1	159.29(10)	C4	C2	C1	110.2(3)
C14	Gd1	O4[1]	78.34(10)	C4	C2	C3	110.0(3)
C14	Gd1	O5	105.63(10)	C2	C3	O2	110.9(3)
C14	Gd1	O7	124.99(10)	C2	C4	O3	110.3(3)
C14	Gd1	O8	73.79(10)	C6	C5	N1	111.5(3)
C14	Gd1	O9	25.60(10)	C7	C6	C5	115.5(3)
C14	Gd1	O10	25.50(10)	C6	C7	N2	110.7(3)
C14	Gd1	O11	96.56(10)	C9	C8	N2	110.0(3)
C14	Gd1	O12	106.42(10)	C10	C8	N2	112.7(3)
C14	Gd1	C12	99.35(11)	C10	C8	C9	107.7(3)
C16	Gd1	Cu1	114.25(8)	C11	C8	N2	105.0(3)
C16	Gd1	Cu2	132.94(8)	C11	C8	C9	109.8(3)

C16	Gd1	O1	81.09(10)	C11	C8	C10	111.6(3)
C16	Gd1	O4[1]	110.39(10)	C8	C9	O6	110.6(3)
C16	Gd1	O5	150.30(9)	C8	C10	O4	115.3(3)
C16	Gd1	O7	98.71(10)	C8	C11	O5	110.5(3)
C16	Gd1	O8	104.55(10)	O7	C12	Gd1	60.9(2)
C16	Gd1	O9	128.02(10)	O8	C12	Gd1	59.01(19)
C16	Gd1	O10	76.93(10)	O8	C12	O7	119.9(4)
C16	Gd1	O11	26.62(10)	C13	C12	Gd1	178.5(3)
C16	Gd1	O12	26.54(10)	C13	C12	O7	120.2(4)
C16	Gd1	C12	103.26(11)	C13	C12	O8	119.9(4)
C16	Gd1	C14	102.42(11)	O9	C14	Gd1	64.5(2)
Cu2[1]	Cu1	Gd1	66.855(9)	O10	C14	Gd1	56.1(2)
O1	Cu1	Gd1	42.34(7)	O10	C14	O9	120.6(4)
O1	Cu1	Cu2[1]	86.25(7)	C15	C14	Gd1	174.0(3)
O2	Cu1	Gd1	100.31(7)	C15	C14	O9	120.9(4)
O2	Cu1	Cu2[1]	58.47(6)	C15	C14	O10	118.5(4)
O2	Cu1	O1	79.88(10)	O11	C16	Gd1	61.3(2)
O5	Cu1	Gd1	46.75(7)	O12	C16	Gd1	58.83(19)
O5	Cu1	Cu2[1]	43.61(7)	O12	C16	O11	120.1(4)
O5	Cu1	O1	87.14(10)	C17	C16	Gd1	177.4(3)
O5	Cu1	O2	101.58(9)	C17	C16	O11	119.7(4)
N1	Cu1	Gd1	128.40(10)	C17	C16	O12	120.2(4)

Table S4. Atomic Occupancy for {Cu_3-Gd_2}.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
O13	0.500000	H13d	0.500000	H13e	0.500000

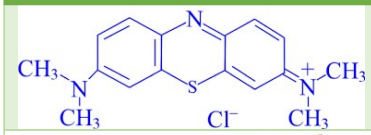
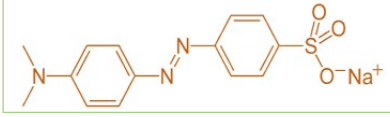
Table S5. Solvent masks information for {Cu_3-Gd_2}.

Number	**X**	**Y**	**Z**	**Volume**	**Electron count**	**Content**
1	0.000	0.000	0.500	159.7	21.1	?
2	0.500	0.500	1.000	159.7	21.1	?

Table S6. Parameters for different kinetic models for adsorption studies of MB and MO.

Model	Pseudo-first order				Pseudo-second order				Intraparticle diffusion	
Parameter	**K_1** (min^{-1})	**qe** (cal) (mg/g)	**qe** (exp) (mg/g)	**R^2**	**k_2** (g /mg min^{-1})	**qe** (cal) (mg/g)	**qe** (exp) (mg/g)	**R^2**	**K_3** (mg /g $min^{-1/2}$)	**R^2**
MB	0.0027	87.5	93.6	0.955	0.0084	98.2	93.6	0.995	10.887	0.956
MO	0.0029	65.13	67.4	0.899	0.008	66.66	67.4	0.993	11.731	0.921

Table S7. Chemical structure and electrical property of dyes used

Structure of dyes	Dye	Molecular formula	Molar mass (g/ mol)	λ_{max} (nm)	Electrical property
	MB	$C_{16}H_{18}ClN_3S$	319.85	665	Cationic
	MO	$C_{14}H_{14}N_3NaO_3S$	327.33	465	Anionic

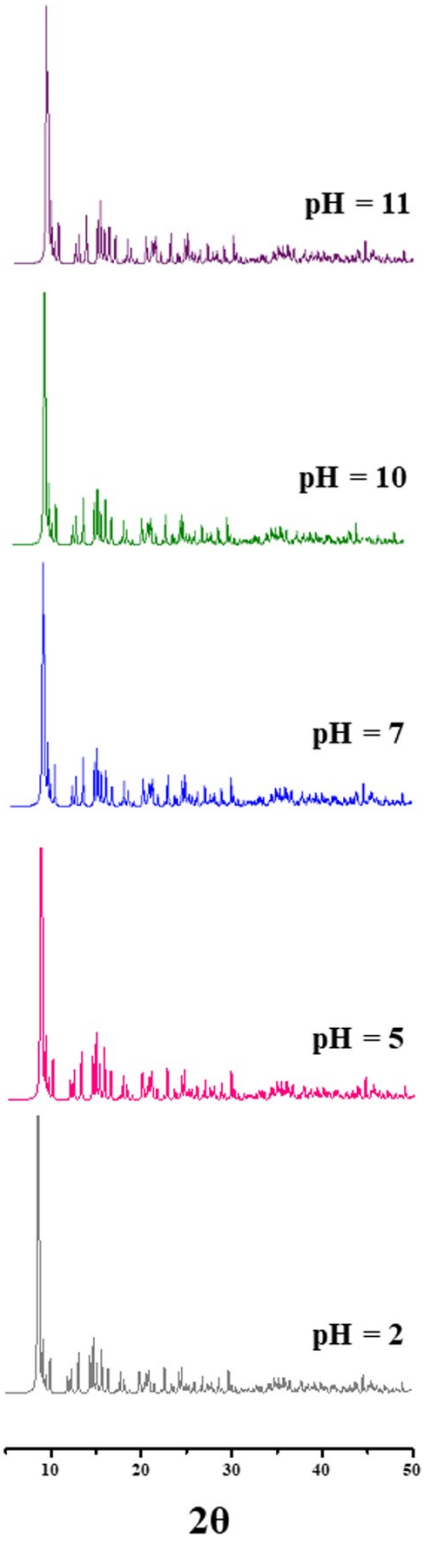


Figure S1. PXRD patterns of **{Cu_3-Gd_2}**@MB after dye adsorption at different pH.