

Supporting Information (SI)

A Water-Stable Cl@Ag₁₄ Cluster Based Metal-Organic Open Framework for Dichromate Trapping and Bacterial Inhibition

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Materials and Instruments

All reagents employed were commercially available and used as received without further purification. The solvents were purified and distilled by standard procedures prior to use. The Raman spectra of compounds in solid state were recorded on a LabRAM HR800 (HORIBA Jobin Yvon) in the frequency range of 50-2500 cm⁻¹. IR spectra were recorded on a PerkinElmer Spectrum Two in the frequency range of 4000-400 cm⁻¹. C, N, and H analyses were performed on an EA1110 CHNS-0 CE 65 elemental analyzer. Energy-dispersive X-ray spectrum was measured using a SU-8010 field emission scanning electron microscope (FESEM; Hitachi Ltd., Tokyo, Japan) equipped with an Oxford-Horiba Inca XMax50 energy-dispersive X-ray (EDX; Oxford Instruments Analytical, High Wycombe, England). Powder X-ray diffraction (PXRD) data were collected on a Philips X’Pert Pro MPD X-ray diffractometer with CuK α radiation equipped with an X’Celerator detector. The diffuse-reflectance spectra were recorded on a UV/Vis spectrophotometer (Evolution 220, ISA-220 accessory, Thermo Scientific) using a built-in 10 mm silicon photodiode with a 60 mm Spectralon sphere. The emission spectra were recorded on a Lumina Fluorescence Spectrometer (Thermo Fisher). Time-resolved photoluminescence lifetime measurements were measured on Edinburgh spectrofluorimeter (F920S) using a time-correlated single-photon counting technique and solid-state quantum yields were determined on an Edinburgh FLS920 fluorescence spectrophotometer equipped with an integrating sphere. The high-resolution electrospray mass spectrometry was performed on an Agilent (Santa Clara, CA, USA) ESI-TOF mass spectrometer (6224).

X-ray Crystallography

Single crystals of **SD/Ag14**, **SD/Ag15** and **SD/Ag16** of appropriate dimensions were chosen under an optical microscope and quickly coated with high vacuum grease (Dow Corning Corporation) to prevent decomposition. Intensity data and cell parameters were recorded at 173 K on a Bruker Apex II single crystal diffractometer, employing a Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) and a CCD area detector. The raw frame data were processed using SAINT and SADABS to yield the reflection data file.¹ The structure was solved using the charge-flipping algorithm, as implemented in the program *SUPERFLIP*² and refined by full-matrix least-squares techniques against F_o^2 using the SHELXL program³ through the OLEX2 interface.⁴ Hydrogen atoms at carbon were placed in calculated positions and refined isotropically by using a riding model. Appropriate restraints or constraints were applied to the geometry and the atomic displacement parameters of the atoms in the cluster. All structures were examined using the Addsym subroutine of PLATON⁵ to ensure that no additional symmetry could be applied to the models. Pertinent crystallographic data collection and refinement parameters are collated in Table S1. Selected bond lengths and angles are collated in Table S2.

Anion Exchange

(a) Molar ratio 2:1 (SD/Ag14 to K₂Cr₂O₇)

Compound **SD/Ag14** (2.9 mg) was immersed into a 2 mL aqueous solution containing 0.176 mg K₂Cr₂O₇ in a sealed cuvette, and the mixture was mildly shaken at room temperature. The anion exchange process was monitored by UV-Vis spectroscopy based on typical absorption of Cr₂O₇²⁻ at 257 nm. The anion exchange capacity of compound **SD/Ag14** was evaluated by measuring the decolorizing rate of aqueous K₂Cr₂O₇ solution, which was calculated by the following formula:

$$D_t = \frac{C_o - C_t}{C_o} \times 100\% = \frac{A_o - A_t}{A_o} \times 100\%$$

Where D_t is absorption efficiency and C_o and A_o and C_t and A_t are the concentration and absorbance of aqueous K₂Cr₂O₇ solution at the peak of 257 nm before and after anion exchange, respectively.

(b) Molar ratio 4:1 (SD/Ag14 to K₂Cr₂O₇)

Compound **SD/Ag14** (5.9 mg) was immersed into a 2 mL aqueous solution containing 0.176 mg K₂Cr₂O₇ in a sealed cuvette, and the mixture was mildly shaken at room temperature. The anion exchange process was monitored by UV-Vis spectroscopy based on typical absorption of Cr₂O₇²⁻ at 257 nm. The adsorption intensity of solution decreases from 1.600 to 0.805 with continuous exchange in 48 h, which means 49.7 % Cr₂O₇²⁻ were exchanged into the cationic framework.

(c) Molar ratio 10:1 (SD/Ag14 to K₂Cr₂O₇)

Compound **SD/Ag14** (14.7 mg) was immersed into a 2 mL aqueous solution containing 0.176 mg K₂Cr₂O₇ in a sealed cuvette, and the mixture was mildly shaken at room temperature. The anion exchange process was monitored by UV-Vis spectroscopy based on typical absorption of Cr₂O₇²⁻ at 257 nm. After 48 h, the solid in the solution was filtered, rinsed with deionized water and dried in air. The resultant solid was used for Raman (Figure S1) and EDS Mapping (Figure S11) measurement. The filtrate was used for HRESI-MS analysis (Figure S9).

(d) Selective capture of Cr₂O₇²⁻

Compound **SD/Ag14** (2.9 mg) was immersed into a 2 mL aqueous solution containing 0.176 mg K₂Cr₂O₇ and salts of NaSO₄ (0.085 mg, 0.0006 mmol), NaClO₄ (0.168 mg, 0.0012 mmol), and

KNO_3 (0.12 mg, 0.0012 mmol) in a sealed cuvette. The anion exchange process was monitored by UV-Vis spectroscopy based on typical absorption of $\text{Cr}_2\text{O}_7^{2-}$ at 257 nm.

Antibacterial measurements

The antibacterial performance of **SD/Ag14** was investigated by the using of the Gram-positive bacteria of *Staphylococcus aureus* (*S. aureus*) as model bacteria to count the visible bacteria colonies. *S. aureus* was cultured in nutrient broth at 37 °C for 12 h with a mechanical shaker. Then cultured bacterial sample was diluted to a cell suspension of 10⁶ CFU/mL. 100 µL of diluted bacterial suspension was taken individually to mix into 100 mL of nutrient broth with and without **SD/Ag14**. The concentration of **SD/Ag14** in nutrient broth was adjusted to 0.1, 1, 5 and 10 µg/mL, respectively. The mixture with no addition of **SD/Ag14** worked as control. Each type of samples had three parallel samples for accuracy and statistic analysis. All the samples were continuously cultured at 37 °C for 12 h. The numbers of survived colonies were counted by diluting the cultured samples into an appropriate concentration and incubating on nutrient agar plates for another 12 h at 37 °C. The significance of any difference between different samples was calculated by a Student's t-test and the difference referred to be significant is a value P < 0.05. The images of bacterial colonies were taken by camera. The bacterial visibility is defined by the following formula:

$$\text{Bacterial visibility (\%)} = \frac{A_t}{A_0} \times 100\%$$

where A_t is the colony number of treated bacteria and A₀ is the colony number of control bacteria.

Table S1: Crystal Data Collection and Structure Refinement for SD/Ag14-SD/Ag16.

Compound	SD/Ag14	SD/Ag15	SD/Ag16
Empirical formula	C ₁₇₁ H ₁₇₃ Ag ₄₂ Cl ₉ O ₁₀ S ₃	C ₁₁₂ H ₁₃₆ Ag ₁₆ O ₂₈ S ₈	C ₁₅₀ H ₁₅₀ Ag ₄₂ Cr ₆ Cl ₉ O ₂₁
Formula weight	7333.93	3912.61	7450.30
Temperature/K	173.15	173.15	173.15
Crystal system	trigonal	triclinic	trigonal
Space group	<i>R</i> -3	<i>P</i> -1	<i>R</i> -3
a/Å	40.383(5)	13.383(6)	40.442(4)
b/Å	40.383(5)	19.107(9)	40.442(4)
c/Å	22.259(3)	27.092(13)	43.406(5)
α/°	90.00	96.298(5)	90
β/°	90.00	99.390(5)	90
γ/°	120.00	109.615(4)	120
Volume/Å ³	31436(6)	6336(5)	61481(15)
Z	6	2	12
ρ _{calc} g/cm ³	2.324	2.051	2.205
μ/mm ⁻¹	4.008	2.610	4.057
F(000)	20712.0	3824.0	38124.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5 to 50	5 to 55.4	3.462 to 49.998
Index ranges	-47 ≤ h ≤ 39, -28 ≤ k ≤ 28, -26 ≤ l ≤ 14	-17 ≤ h ≤ 17, -24 ≤ k ≤ 24, -35 ≤ l ≤ 35	-30 ≤ h ≤ 44, -48 ≤ k ≤ 27, -51 ≤ l ≤ 51
Reflections collected	25449	74001	60762
Independent reflections	12257 [R _{int} = 0.0744, R _{sigma} = 0.1480]	29262 [R _{int} = 0.0367, R _{sigma} = 0.0473]	24010 [R _{int} =0.1178, R _{sigma} = 0.1942]
Data/parameters	12257/639	29262/1517	24010/1207
Goodness-of-fit on F ²	0.900	1.013	0.999
Final R indexes [I>=2σ (I)]	R ₁ = 0.0609, wR ₂ = 0.1301	R ₁ = 0.0388, wR ₂ = 0.0859	R ₁ = 0.0780, wR ₂ = 0.1811
Final R indexes [all data]	R ₁ = 0.1370, wR ₂ = 0.1499	R ₁ = 0.0671, wR ₂ = 0.0983	R ₁ = 0.2183, wR ₂ = 0.2591
Largest diff. peak/hole/eÅ ⁻³	1.63/-1.64	3.67/-1.56	1.36/-1.04

Table S2: Selected bond lengths (Å) and angles (°) for SD/Ag14-SD/Ag16.

Compound SD/Ag14			
Ag14—Ag10	3.1798 (16)	Ag1—Ag6 ⁱⁱ	2.9959 (17)
Ag14—Ag11	3.1972 (15)	Ag1—C1	2.11 (2)
Ag14—Ag13	2.9855 (16)	Ag1—C11	2.148 (18)
Ag14—Ag12	2.9087 (16)	Ag7—Ag2 ⁱ	3.2522 (18)
Ag14—Cl2 ⁱ	2.879 (3)	Ag7—Ag1 ⁱ	2.9140 (17)
Ag14—C46	2.152 (17)	Ag7—Ag6	3.3259 (18)
Ag14—C41	2.256 (17)	Ag7—Ag9	2.9176 (17)
Ag14—C42	2.573 (17)	Ag7—C1 ⁱ	2.381 (17)
Ag10—Ag11	2.8630 (15)	Ag7—C6 ⁱ	2.38 (2)
Ag10—Ag8	3.2300 (16)	Ag7—C31	2.372 (15)
Ag10—Ag9	3.0551 (16)	Ag8—Ag9	3.0992 (17)
Ag10—Cl2	2.736 (3)	Ag8—Cl2	2.847 (3)
Ag10—Cl3	2.800 (4)	Ag8—C21	2.481 (16)
Ag10—C41	2.306 (14)	Ag8—C36	2.367 (18)
Ag10—C36	2.325 (16)	Ag8—C31	2.363 (14)
Ag3—Ag11 ⁱⁱ	3.0102 (16)	Ag4—Ag1 ⁱⁱⁱ	3.0863 (17)
Ag3—Ag5	3.1243 (16)	Ag4—Ag12 ⁱⁱ	3.1569 (16)
Ag3—Ag2	3.2014 (17)	Ag4—Cl1	2.688 (4)
Ag3—Ag8	3.0433 (16)	Ag4—C21	2.456 (15)
Ag3—Ag4	2.9358 (17)	Ag4—C1 ⁱⁱⁱ	2.570 (15)
Ag3—Ag12 ⁱⁱ	3.0500 (17)	Ag4—C11	2.305 (16)
Ag3—C21	2.133 (15)	Ag6—Ag1 ⁱ	2.9958 (17)
Ag3—C16	2.075 (16)	Ag6—Cl1 ⁱ	2.579 (4)
Ag11—Ag3 ⁱ	3.0101 (16)	Ag6—C26	2.413 (17)
Ag11—Ag5 ⁱ	3.0761 (15)	Ag6—C1 ⁱ	2.306 (15)
Ag11—Ag13 ⁱ	3.1935 (16)	Ag13—Ag11 ⁱⁱ	3.1932 (16)
Ag11—C41	2.165 (15)	Ag13—Cl2	2.675 (4)
Ag11—C26 ⁱ	2.560 (17)	Ag13—C46	2.280 (17)
Ag11—C16 ⁱ	2.230 (14)	Ag13—C26	2.462 (16)
Ag5—Ag11 ⁱⁱ	3.0759 (16)	Ag12—Ag3 ⁱ	3.0499 (17)
Ag5—Ag7	3.0159 (16)	Ag12—Cl1 ⁱ	2.718 (4)
Ag5—Ag8	3.1453 (17)	Ag12—C21 ⁱ	2.334 (15)
Ag5—Ag6	2.9821 (17)	Ag12—C46	2.287 (19)
Ag5—Ag13	3.2678 (16)	Ag9—Ag2 ⁱ	3.1324 (17)
Ag5—C26	2.107 (18)	Ag9—C36	2.080 (19)
Ag5—C31	2.083 (17)	Ag9—C6 ⁱ	2.11 (2)
Ag2—Ag1	2.9668 (17)	Cl2—Ag14 ⁱⁱ	2.878 (3)
Ag2—Ag7 ⁱⁱ	3.2520 (18)	Cl3—Ag2 ⁱ	2.777 (4)
Ag2—Ag9 ⁱⁱ	3.1324 (17)	Cl1—Ag6 ⁱⁱ	2.579 (4)

Ag2—Cl3 ⁱⁱ	2.777 (4)	Cl1—Ag12 ⁱⁱ	2.718 (4)
Ag2—C17	2.544 (17)	C21—Ag12 ⁱⁱ	2.334 (15)
Ag2—C16	2.413 (14)	C26—Ag11 ⁱⁱ	2.559 (17)
Ag2—C11	2.401 (14)	C16—Ag11 ⁱⁱ	2.230 (14)
Ag2—C6	2.38 (2)	C1—Ag7 ⁱⁱ	2.381 (17)
Ag1—Ag1 ⁱⁱⁱ	3.268 (2)	C1—Ag4 ⁱⁱⁱ	2.570 (15)
Ag1—Ag7 ⁱⁱ	2.9140 (17)	C1—Ag6 ⁱⁱ	2.306 (15)
Ag1—Ag4	2.9688 (18)	C6—Ag7 ⁱⁱ	2.38 (2)
Ag1—Ag4 ⁱⁱⁱ	3.0863 (17)	C6—Ag9 ⁱⁱ	2.11 (2)
C46—Ag14—Cl2 ⁱ	102.4 (5)	C1—Ag1—C11	173.1 (6)
C46—Ag14—C41	169.5 (6)	C1 ⁱ —Ag7—C6 ⁱ	126.5 (7)
C46—Ag14—C42	147.7 (6)	C1 ⁱ —Ag7—C31	112.8 (6)
C41—Ag14—Cl2 ⁱ	87.8 (4)	C6 ⁱ —Ag7—C31	118.3 (7)
C41—Ag14—C42	27.1 (5)	C21—Ag8—Cl2	90.8 (3)
C42—Ag14—Cl2 ⁱ	91.9 (3)	C36—Ag8—Cl2	94.7 (4)
Cl2—Ag10—Cl3	87.28 (10)	C36—Ag8—C21	127.4 (6)
C41—Ag10—Cl2	102.4 (4)	C36—Ag8—C31	119.6 (6)
C41—Ag10—Cl3	106.9 (4)	C31—Ag8—Cl2	110.1 (4)
C41—Ag10—C36	134.7 (6)	C31—Ag8—C21	107.0 (5)
C36—Ag10—Cl2	98.6 (5)	C21—Ag4—Cl1	91.0 (4)
C36—Ag10—Cl3	113.8 (5)	C21—Ag4—C1 ⁱⁱⁱ	117.5 (5)
C16—Ag3—C21	175.0 (6)	C1 ⁱⁱⁱ —Ag4—Cl1	94.8 (4)
C41—Ag11—C26 ⁱ	108.5 (5)	C11—Ag4—Cl1	133.7 (4)
C41—Ag11—C16 ⁱ	157.4 (5)	C11—Ag4—C21	126.2 (5)
C16 ⁱ —Ag11—C26 ⁱ	94.0 (5)	C11—Ag4—C1 ⁱⁱⁱ	90.9 (5)
C31—Ag5—C26	167.9 (6)	C26—Ag6—Cl1 ⁱ	108.2 (4)
C17—Ag2—Cl3 ⁱⁱ	108.4 (4)	C1 ⁱ —Ag6—Cl1 ⁱ	126.8 (5)
C16—Ag2—C17	27.9 (4)	C46—Ag13—Cl2	123.7 (4)
C11—Ag2—Cl3 ⁱⁱ	106.3 (4)	C46—Ag13—C26	132.6 (6)
C11—Ag2—C17	118.5 (6)	C26—Ag13—Cl2	103.6 (4)
C11—Ag2—C16	105.9 (5)	C21 ⁱ —Ag12—Cl1 ⁱ	93.0 (4)
C6—Ag2—Cl3 ⁱⁱ	101.5 (5)	C46—Ag12—Cl1 ⁱ	109.6 (4)
C6—Ag2—C17	105.6 (7)	C46—Ag12—C21 ⁱ	150.4 (5)
C6—Ag2—C16	131.5 (7)	C36—Ag9—C6 ⁱ	175.9 (8)
C6—Ag2—C11	115.1 (6)		

Symmetry codes: (i) $x-y+2/3, x+1/3, -z+4/3$; (ii) $y-1/3, -x+y+1/3, -z+4/3$; (iii) $-x+1, -y+1, -z+1$.

Compound SD/Ag15

Ag4—Ag6	2.9481 (10)	Ag11—Ag10	3.2701 (17)
Ag4—Ag8	3.2813 (17)	Ag11—O18	2.354 (4)
Ag4—Ag5	3.0628 (10)	Ag11—C5	2.354 (5)
Ag4—Ag7	2.8094 (10)	Ag11—C40	2.288 (5)
Ag4—Ag3	2.9247 (11)	Ag11—C4	2.675 (6)

Ag4—Ag2	2.9192 (12)	Ag9—O11	2.389 (3)
Ag4—Ag1	2.9096 (11)	Ag9—C25	2.357 (5)
Ag4—C20	2.096 (5)	Ag9—C35	2.306 (5)
Ag4—C15	2.100 (5)	Ag9—O2 ⁱ	2.575 (4)
Ag6—Ag8	3.0843 (10)	Ag7—O9	2.378 (4)
Ag6—Ag7	3.3389 (17)	Ag7—O4	2.507 (4)
Ag6—C20	2.357 (5)	Ag7—C15	2.407 (5)
Ag6—O10	2.348 (4)	Ag7—C35	2.433 (5)
Ag6—C35	2.310 (5)	Ag13—O8	2.321 (4)
Ag8—Ag12	3.3098 (17)	Ag13—C10	2.454 (5)
Ag8—Ag5	3.0108 (10)	Ag13—C5	2.305 (5)
Ag8—Ag11	3.0188 (10)	Ag13—O1 ⁱ	2.405 (4)
Ag8—Ag9	3.0077 (10)	Ag14—O15	2.272 (4)
Ag8—Ag7	3.0066 (10)	Ag14—O28	2.432 (4)
Ag8—Ag10	2.9872 (10)	Ag14—C5	2.460 (5)
Ag8—C40	2.137 (5)	Ag14—C30	2.386 (5)
Ag8—C35	2.127 (5)	Ag10—O14	2.413 (4)
Ag12—Ag11	2.9489 (10)	Ag10—O22	2.393 (4)
Ag12—Ag9	3.0143 (10)	Ag10—C40	2.449 (5)
Ag12—Ag13	2.9599 (12)	Ag10—C25	2.454 (5)
Ag12—Ag14	2.8936 (12)	Ag3—Ag15 ⁱⁱ	2.9786 (13)
Ag12—Ag10	2.8325 (10)	Ag3—C20	2.286 (5)
Ag12—Ag16	2.9127 (11)	Ag3—O21	2.311 (4)
Ag12—C5	2.106 (5)	Ag3—C29 ⁱⁱ	2.671 (5)
Ag12—C25	2.105 (5)	Ag3—O19	2.386 (4)
Ag5—Ag11	3.3364 (17)	Ag3—C30 ⁱⁱ	2.476 (5)
Ag5—O16	2.422 (4)	Ag2—Ag15 ⁱⁱ	2.8659 (14)
Ag5—O20	2.513 (4)	Ag2—C20	2.490 (5)
Ag5—C15	2.374 (5)	Ag2—O3	2.461 (4)
Ag5—C40	2.305 (5)	Ag2—C10 ⁱⁱ	2.389 (5)
Ag15—Ag13	2.9710 (13)	Ag2—O5	2.261 (4)
Ag15—Ag14	2.8489 (14)	Ag16—O24	2.354 (5)
Ag15—Ag3 ⁱ	2.9786 (13)	Ag16—C25	2.414 (5)
Ag15—Ag2 ⁱ	2.8659 (14)	Ag16—C30	2.273 (5)
Ag15—Ag16	3.2108 (14)	Ag1—Ag15 ⁱⁱ	3.1870 (14)
Ag15—Ag1 ⁱ	3.1870 (14)	Ag1—C10 ⁱⁱ	2.269 (5)
Ag15—C10	2.133 (5)	Ag1—C15	2.481 (5)
Ag15—C30	2.132 (5)	Ag1—O25	2.328 (5)
C20—Ag4—C15	170.28 (18)	C5—Ag13—O1 ⁱ	126.69 (17)
O10—Ag6—C20	116.78 (15)	O1 ⁱ —Ag13—C10	94.44 (16)
C35—Ag6—C20	135.80 (17)	O15—Ag14—C5	108.94 (15)
C35—Ag6—O10	106.50 (15)	O15—Ag14—C30	125.08 (17)
C35—Ag8—C40	178.05 (18)	O28—Ag14—C5	96.77 (15)

C25—Ag12—C5	167.5 (2)	C30—Ag14—O28	92.62 (15)
O16—Ag5—O20	75.82 (12)	C30—Ag14—C5	118.03 (16)
C15—Ag5—O16	118.33 (15)	O14—Ag10—C40	111.60 (14)
C15—Ag5—O20	82.52 (15)	O14—Ag10—C25	96.62 (16)
C40—Ag5—O16	107.57 (15)	O22—Ag10—O14	108.67 (13)
C40—Ag5—O20	123.74 (15)	O22—Ag10—C40	99.28 (14)
C40—Ag5—C15	131.98 (16)	O22—Ag10—C25	109.70 (15)
C30—Ag15—C10	178.38 (19)	C40—Ag10—C25	130.17 (17)
O18—Ag11—C5	114.67 (15)	C20—Ag3—O21	113.77 (15)
O18—Ag11—C4	88.80 (16)	C20—Ag3—O19	135.29 (17)
C5—Ag11—C4	26.54 (17)	O21—Ag3—O19	88.63 (13)
C40—Ag11—O18	105.18 (15)	O21—Ag3—C30 ⁱⁱ	119.10 (15)
C40—Ag11—C5	139.72 (17)	O19—Ag3—C29 ⁱⁱ	84.66 (16)
C40—Ag11—C4	166.02 (17)	O19—Ag3—C30 ⁱⁱ	91.55 (15)
O11—Ag9—O2 ⁱ	75.05 (12)	C30 ⁱⁱ —Ag3—C29 ⁱⁱ	27.06 (15)
C25—Ag9—O11	116.24 (16)	O3—Ag2—C20	97.09 (14)
C25—Ag9—O2 ⁱ	81.57 (15)	C10 ⁱⁱ —Ag2—C20	114.18 (16)
C35—Ag9—O11	109.31 (15)	C10 ⁱⁱ —Ag2—O3	89.60 (15)
C35—Ag9—C25	131.97 (17)	O5—Ag2—C20	110.59 (15)
C35—Ag9—O2 ⁱ	125.79 (15)	O5—Ag2—O3	110.82 (13)
O9—Ag7—O4	107.20 (13)	O5—Ag2—C10 ⁱⁱ	127.50 (16)
O9—Ag7—C15	112.81 (15)	O24—Ag16—C25	112.79 (17)
O9—Ag7—C35	100.93 (15)	C30—Ag16—O24	116.96 (17)
C15—Ag7—O4	98.10 (15)	C30—Ag16—C25	124.28 (18)
C35—Ag7—O4	106.69 (14)	C10 ⁱⁱ —Ag1—C15	122.18 (17)
O8—Ag13—O1 ⁱ	90.56 (14)	C10 ⁱⁱ —Ag1—O25	121.30 (18)
C5—Ag13—O8	113.34 (16)	O25—Ag1—C15	108.20 (17)
C5—Ag13—C10	111.19 (17)		

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$.

Compound SD/Ag16

Ag1—C1	2.17 (3)	Ag16—Cl4	2.529 (6)
Ag1—C2 ⁱ	2.33 (4)	Ag16—Ag27 ⁱⁱⁱ	2.908 (3)
Ag1—C93 ⁱ	2.60 (4)	Ag16—Ag17	3.043 (3)
Ag1—Cl1 ⁱ	2.759 (6)	Ag16—Ag28	3.188 (3)
Ag1—Cl2 ⁱ	2.844 (6)	Ag17—C32	2.06 (3)
Ag1—Ag12	2.857 (3)	Ag17—C31	2.15 (3)
Ag1—Ag2	3.063 (3)	Ag17—Ag28	2.884 (3)
Ag1—Ag3 ⁱ	3.140 (3)	Ag17—Ag18	3.002 (3)
Ag1—Ag4 ⁱ	3.160 (3)	Ag18—C36 ⁱⁱⁱ	2.33 (4)
Ag2—C1	2.25 (3)	Ag18—C32	2.37 (3)
Ag2—C97	2.56 (4)	Ag18—C33	2.44 (2)
Ag2—Cl1	2.894 (6)	Ag18—C64	2.67 (3)
Ag2—Ag11 ⁱ	2.942 (3)	Ag18—Cl6 ⁱⁱⁱ	2.771 (6)

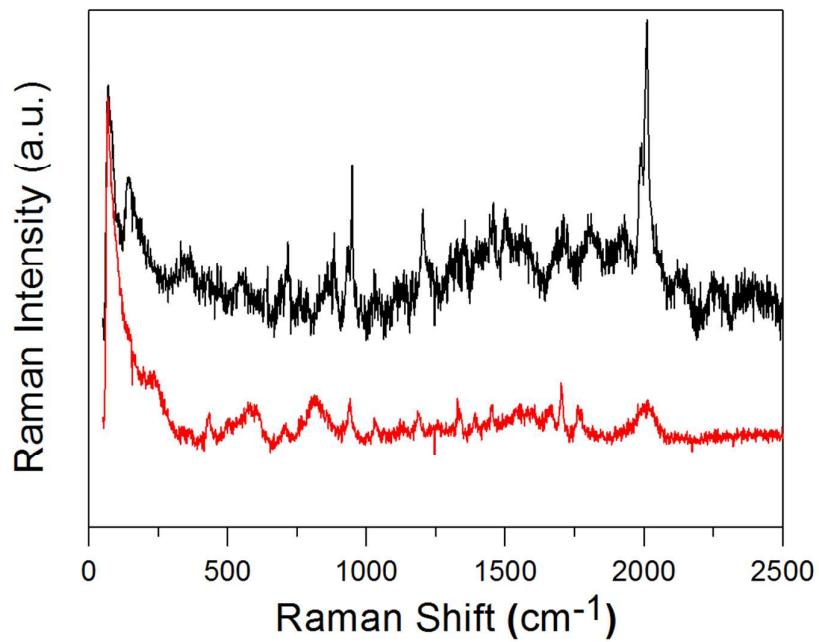
Ag2—Ag6 ⁱ	2.952 (3)	Ag18—Ag22 ⁱⁱⁱ	3.062 (3)
Ag2—Ag12	3.207 (3)	Ag18—Ag19	3.122 (3)
Ag3—C2	2.29 (4)	Ag18—Ag28	3.297 (3)
Ag3—C22	2.33 (3)	Ag19—C34	2.12 (2)
Ag3—C4 ⁱ	2.51 (3)	Ag19—C33	2.17 (2)
Ag3—C10 ⁱ	2.71 (3)	Ag19—Ag24	2.968 (2)
Ag3—Cl1	2.779 (7)	Ag19—Ag25	3.065 (3)
Ag3—Ag4	2.919 (3)	Ag19—Ag20	3.079 (3)
Ag3—Ag1 ⁱⁱ	3.140 (3)	Ag19—Ag27	3.115 (3)
Ag3—Ag8 ⁱ	3.167 (3)	Ag20—C72 ^{iv}	2.32 (3)
Ag4—C2	2.12 (4)	Ag20—C35	2.33 (2)
Ag4—C3	2.12 (3)	Ag20—C34	2.43 (2)
Ag4—Ag14	2.862 (3)	Ag20—Cl5	2.818 (6)
Ag4—Ag5	3.129 (3)	Ag20—Ag22	3.002 (3)
Ag4—Ag1 ⁱⁱ	3.160 (3)	Ag20—Ag27	3.045 (3)
Ag5—C5	2.34 (3)	Ag20—Ag21	3.235 (3)
Ag5—C3	2.35 (3)	Ag21—C45 ^{iv}	2.30 (3)
Ag5—C14	2.40 (3)	Ag21—C35	2.36 (2)
Ag5—C6	2.54 (3)	Ag21—C41	2.70 (2)
Ag5—Cl2	2.780 (6)	Ag21—Cl5	2.728 (6)
Ag5—Ag9	2.988 (3)	Ag21—Cl6	2.785 (6)
Ag5—Ag8	3.108 (3)	Ag21—Ag24 ^{iv}	2.866 (3)
Ag5—Ag14	3.228 (3)	Ag21—Ag23 ^{iv}	3.085 (3)
Ag6—C17	2.28 (3)	Ag21—Ag22	3.097 (3)
Ag6—C4	2.38 (3)	Ag22—C36	2.05 (5)
Ag6—C18	2.66 (3)	Ag22—C35	2.10 (3)
Ag6—Cl3	2.764 (6)	Ag22—Ag28 ^{iv}	2.886 (3)
Ag6—Ag2 ⁱⁱ	2.952 (3)	Ag22—Ag18 ^{iv}	3.062 (3)
Ag6—Ag8	3.043 (3)	Ag23—C50	2.11 (3)
Ag6—Ag7	3.188 (3)	Ag23—C45	2.26 (2)
Ag7—C14	2.27 (4)	Ag23—C46	2.51 (3)
Ag7—C4	2.40 (3)	Ag23—Ag25	2.891 (3)
Ag7—C31	2.63 (2)	Ag23—Cl5	2.928 (6)
Ag7—Cl3	2.657 (6)	Ag23—Ag21 ⁱⁱⁱ	3.085 (3)
Ag7—Ag9	2.939 (3)	Ag23—Ag26 ⁱⁱⁱ	3.114 (3)
Ag7—Ag8	2.969 (3)	Ag23—Ag24	3.225 (3)
Ag7—Ag17	3.105 (3)	Ag24—C45	2.14 (3)
Ag8—C5	2.08 (3)	Ag24—C33	2.18 (2)
Ag8—C4	2.11 (3)	Ag24—C55	2.68 (3)
Ag8—Ag12 ⁱⁱ	3.009 (3)	Ag24—Ag21 ⁱⁱⁱ	2.865 (3)
Ag8—Ag13 ⁱⁱ	3.089 (3)	Ag24—Ag27	3.121 (3)
Ag8—Ag3 ⁱⁱ	3.167 (3)	Ag24—Ag26	3.143 (3)
Ag9—C14	2.04 (3)	Ag25—C50	2.23 (3)

Ag9—C15	2.11 (3)	Ag25—C34	2.34 (2)
Ag9—Ag14	2.891 (3)	Ag25—Cl4	2.754 (6)
Ag9—Ag10	3.042 (3)	Ag25—Ag26 ⁱⁱⁱ	3.336 (3)
Ag9—Ag15	3.063 (2)	Ag26—C50 ^{iv}	2.32 (3)
Ag9—Ag17	3.307 (3)	Ag26—C55	2.35 (3)
Ag10—C15	2.35 (3)	Ag26—Cl5	2.673 (6)
Ag10—C16	2.35 (4)	Ag26—Ag23 ^{iv}	3.114 (3)
Ag10—Cl3	2.538 (6)	Ag26—Ag27	3.176 (3)
Ag10—Ag13	2.927 (3)	Ag26—Ag25 ^{iv}	3.336 (3)
Ag11—C17	2.22 (3)	Ag27—C72 ^{iv}	2.09 (2)
Ag11—C16	2.41 (3)	Ag27—C55	2.15 (3)
Ag11—Cl1	2.644 (6)	Ag27—Ag16 ^{iv}	2.908 (3)
Ag11—Ag2 ⁱⁱ	2.942 (3)	Ag27—Ag28 ^{iv}	3.040 (3)
Ag11—Ag12	3.209 (3)	Ag28—C36 ⁱⁱⁱ	2.34 (4)
Ag11—Ag13	3.226 (3)	Ag28—C31	2.36 (3)
Ag12—C1	2.11 (3)	Ag28—C72	2.43 (2)
Ag12—C5 ⁱ	2.29 (3)	Ag28—C73	2.68 (3)
Ag12—Ag13	3.055 (3)	Ag28—Ag22 ⁱⁱⁱ	2.887 (3)
Ag13—C22	2.06 (3)	Ag28—Ag27 ⁱⁱⁱ	3.040 (3)
Ag13—C16	2.14 (4)	Cl1—Ag1 ⁱⁱ	2.759 (6)
Ag13—Ag14	3.039 (3)	Cl2—Ag1 ⁱⁱ	2.844 (6)
Ag13—Ag8 ⁱ	3.089 (3)	Cl6—Ag18 ^{iv}	2.770 (6)
Ag14—C3	2.30 (3)	C2—Ag1 ⁱⁱ	2.33 (4)
Ag14—C15	2.35 (3)	C4—Ag3 ⁱⁱ	2.51 (3)
Ag14—C22	2.41 (3)	C5—Ag12 ⁱⁱ	2.29 (3)
Ag14—C23	2.70 (3)	C10—Ag3 ⁱⁱ	2.71 (3)
Ag15—C32	2.22 (3)	C17—Ag2 ⁱⁱ	2.16 (3)
Ag15—C34	2.46 (2)	C36—Ag18 ^{iv}	2.33 (4)
Ag15—C15	2.57 (3)	C36—Ag28 ^{iv}	2.34 (4)
Ag15—Cl4	2.664 (6)	C45—Ag21 ⁱⁱⁱ	2.30 (3)
Ag15—Ag17	2.895 (3)	C50—Ag26 ⁱⁱⁱ	2.32 (3)
Ag15—Ag19	2.926 (2)	C55—Ag16 ^{iv}	2.38 (3)
Ag15—Ag25	3.135 (3)	C72—Ag27 ⁱⁱⁱ	2.09 (2)
Ag16—C31	2.33 (3)	C72—Ag20 ⁱⁱⁱ	2.32 (2)
Ag16—C55 ⁱⁱⁱ	2.38 (3)	C93—Ag1 ⁱⁱ	2.60 (4)
C1—Ag1—C2 ⁱ	135.3(13)	C2 ⁱ —Ag1—Cl2 ⁱ	111.7(10)
C1—Ag1—C93 ⁱ	112.4(13)	C93 ⁱ —Ag1—Cl2 ⁱ	133.1(10)
C2 ⁱ —Ag1—C93 ⁱ	23.1(11)	C11 ⁱ —Ag1—Cl2 ⁱ	86.11(18)
C1—Ag1—Cl1 ¹	106.1(9)	C17 ⁱ —Ag2—C1	172.4(12)
C2 ⁱ —Ag1—Cl1 ⁱ	96.5(9)	C17 ⁱ —Ag2—C97	154.1(11)
C93 ⁱ —Ag1—Cl1 ⁱ	104.2(9)	C36—Ag22—C35	174.3(13)
C1—Ag1—Cl2 ⁱ	108.0(9)	C50—Ag23—C45	173.0(10)
C50—Ag23—C46	148.3(9)	C45—Ag24—C55	109.2(9)

C45—Ag23—C46	29.0(8)	C33—Ag24—C55	92.5(9)
C2—Ag3—C22	131.0(12)	C2—Ag4—C3	178.9(14)
C45 ^{iv} —Ag21—C35	135.6(9)	C2—Ag3—C4 ⁱ	122.7(12)
C45 ^{iv} —Ag21—C41	113.0(8)	C22—Ag3—C4 ⁱ	96.7(10)
C35—Ag21—C41	25.0(7)	C2—Ag3—C10 ⁱ	98.0(12)
C45 ^{iv} —Ag21—Cl5	104.8(7)	C22—Ag3—C10 ⁱ	113.7(10)
C35—Ag21—Cl5	97.0(6)	C4 ⁱ —Ag3—C10 ⁱ	25.5(7)
C41—Ag21—Cl5	96.1(6)	C2—Ag3—Cl1	96.9(10)
C45 ^{iv} —Ag21—Cl6	109.4(6)	C22—Ag3—Cl1	111.5(8)
C35—Ag21—Cl6	110.4(7)	C4 ⁱ —Ag3—Cl1	90.9(7)
C41—Ag21—Cl6	135.4(6)	C10 ⁱ —Ag3—Cl1	101.2(7)
Cl5—Ag21—Cl6	85.63(18)	C50—Ag25—C34	147.7(9)
C1—Ag2—C97	27.3(10)	C50—Ag25—Cl4	111.8(7)
C17 ⁱ —Ag2—Cl1	97.6(8)	C34—Ag25—Cl4	93.4(5)
C1—Ag2—Cl1	89.3(8)	C5—Ag5—C3	132.2(11)
C97—Ag2—Cl1	92.0(7)	C5—Ag5—C14	110.8(12)
C50—Ag23—Cl5	100.5(8)	C3—Ag5—C14	110.9(11)
C45—Ag23—Cl5	86.4(7)	C5—Ag5—C6	28.0(9)
C46—Ag23—Cl5	90.5(6)	C3—Ag5—C6	105.4(10)
C45—Ag24—C33	157.8(10)	C14—Ag5—C6	126.7(12)
C31—Ag7—Cl3	95.1(6)	C5—Ag5—Cl2	90.7(7)
C36 ⁱⁱⁱ —Ag28—C31	126.1(13)	C3—Ag5—Cl2	101.0(8)
C36 ⁱⁱⁱ —Ag28—C72	116.7(13)	C14—Ag5—Cl2	103.8(8)
C31—Ag28—C72	114.7(9)	C6—Ag5—Cl2	106.1(7)
C36 ⁱⁱⁱ —Ag28—C73	103.9(13)	C50 ^{iv} —Ag26—C55	136.1(9)
C31—Ag28—C73	115.5(9)	C50 ^{iv} —Ag26—Cl5	115.7(7)
C72—Ag28—C73	25.8(7)	C55—Ag26—Cl5	107.8(7)
C72 ^{iv} —Ag20—C35	122.8(10)	C17—Ag6—C4	152.9(10)
C72 ^{iv} —Ag20—C34	105.4(9)	C17—Ag6—C18	24.4(8)
C35—Ag20—C34	123.6(9)	C4—Ag6—C18	135.8(10)
C72 ^{iv} —Ag20—Cl5	113.2(6)	C17—Ag6—Cl3	108.8(8)
C35—Ag20—Cl5	95.1(6)	C4—Ag6—Cl3	90.0(6)
C34—Ag20—Cl5	90.5(6)	C18—Ag6—Cl3	99.7(7)
C14—Ag9—C15	172.0(12)	C72 ^{iv} —Ag27—C55	165.7(9)
C4—Ag7—C31	120.6(9)	C5—Ag8—C4	174.3(10)
C14—Ag7—Cl3	130.5(9)	C14—Ag7—C4	126.2(10)
C4—Ag7—Cl3	92.1(7)	C14—Ag7—C31	90.6(10)

Symmetry codes: (i) $y-1/3, -x+y+1/3, -z+4/3$; (ii) $x-y+2/3, x+1/3, -z+4/3$; (iii) $y+1/3, -x+y+2/3, -z+5/3$; (iv) $x-y+1/3, x-1/3, -z+5/3$.

Figure S1: The Raman spectra of SD/Ag14 (black) and SD/Ag16 (red).



Experimental conditions: laser excitation 632.81 nm, 100- μm slits, 298 K.

Figure S2: The IR spectra of SD/Ag14 and SD/Ag15

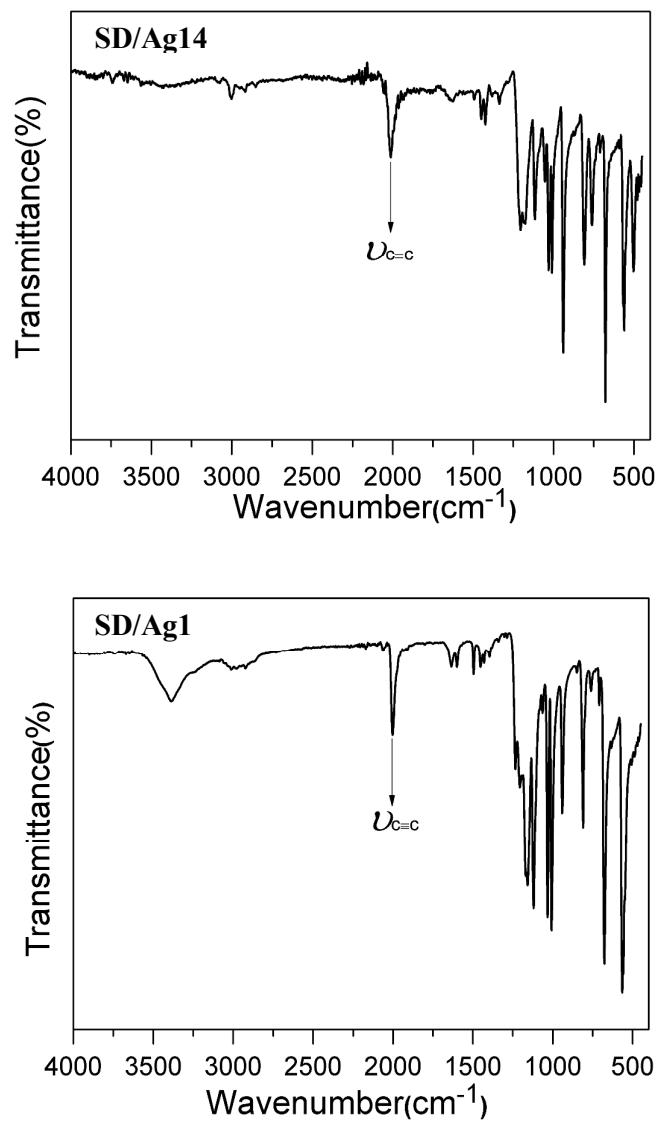


Figure S3: The UV-Vis spectrum of SD/Ag15 in the solid state.

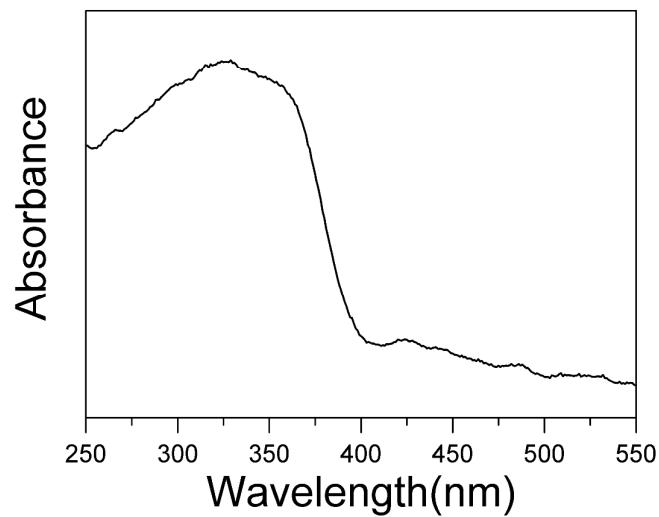


Figure S4: Luminescent lifetime of SD/Ag15 at 293 K (red line is fitting curve).

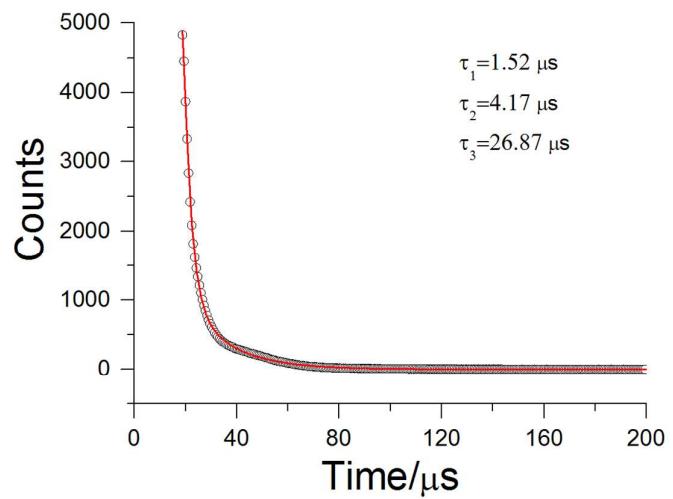


Figure S5: The excitation spectrum of SD/Ag15 in the solid state.

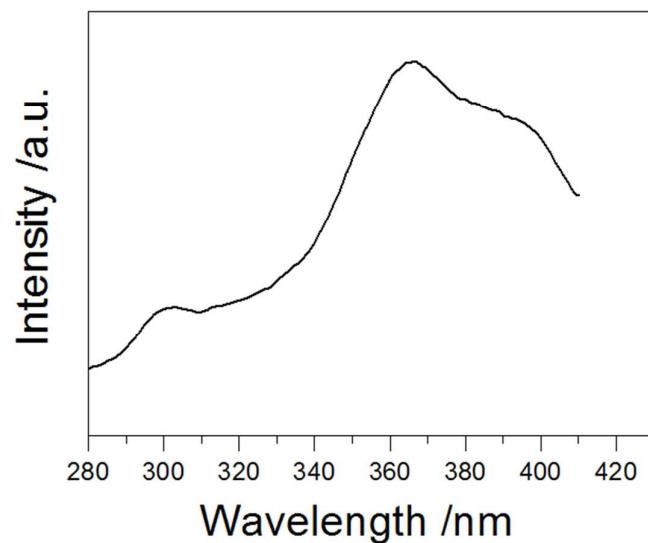


Figure S6: The 3D open framework of SD/Ag14 with its channel filled by *p*-TOS.

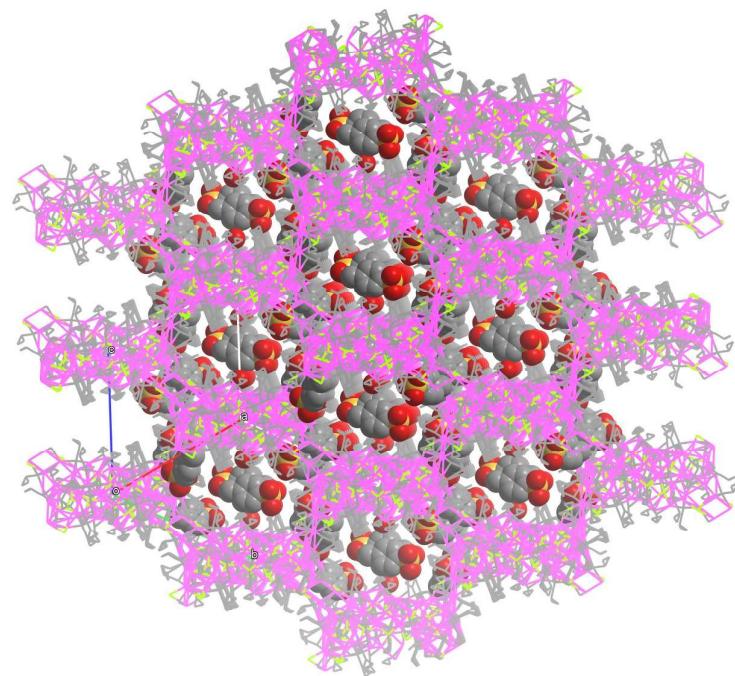
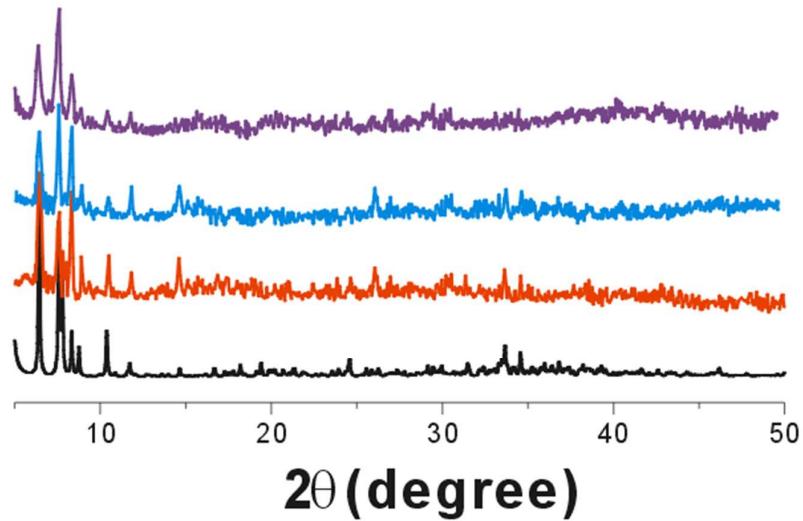


Figure S7: The compared powder X-ray diffraction patterns.



Black: The simulated PXRD pattern of **SD/Ag14**.

Red: The experimental PXRD pattern of microcrystalline sample of **SD/Ag14**.

Cyan: The experimental PXRD pattern of microcrystalline sample of **SD/Ag14** immersed in water for two weeks.

Purple: The experimental PXRD pattern of microcrystalline sample of **SD/Ag14** immersed in $\text{K}_2\text{Cr}_2\text{O}_7$ aqueous solution for two weeks.

Figure S8: The concentration dependent UV-vis absorption data for the capture of dichromate anion. (a) molar ratio of SD/Ag14 and $K_2Cr_2O_7$ = 4:1; (b) molar ratio of SD/Ag14 and $K_2Cr_2O_7$ = 10:1

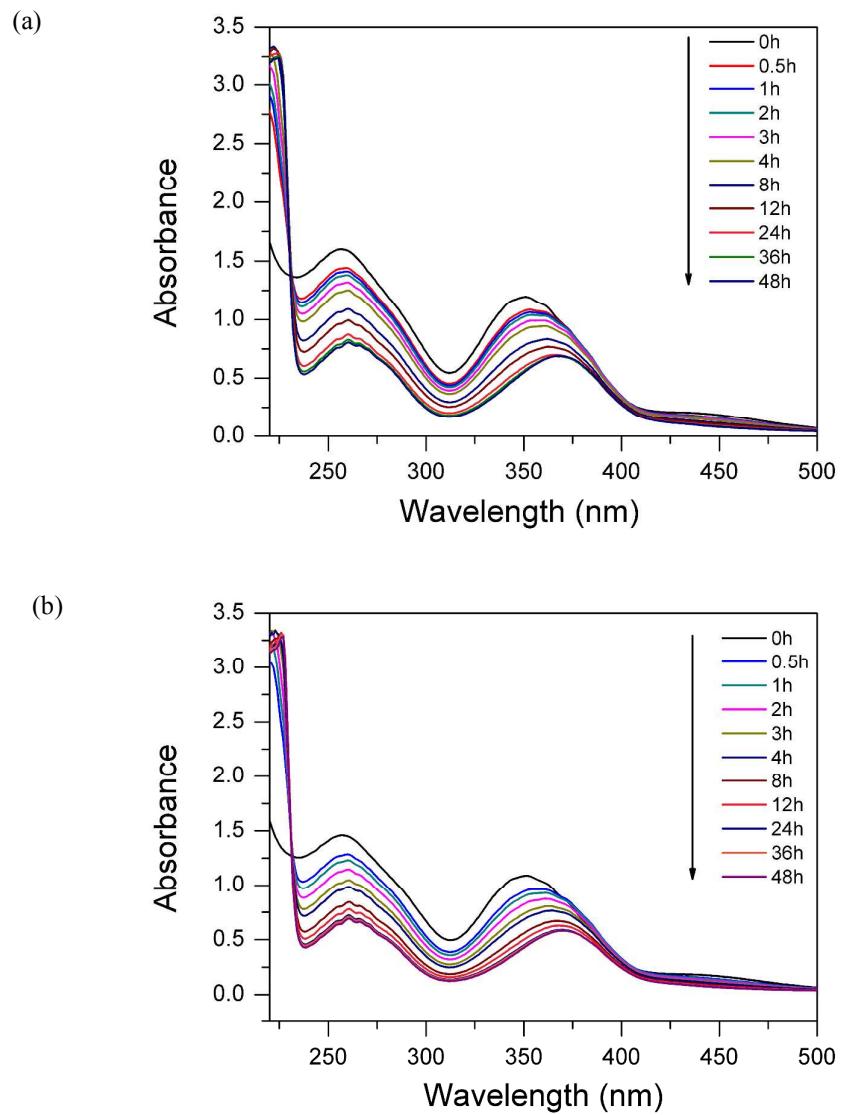


Figure S9: The negative mode HRESI-MS of the solution after anion exchange for SD/Ag14.

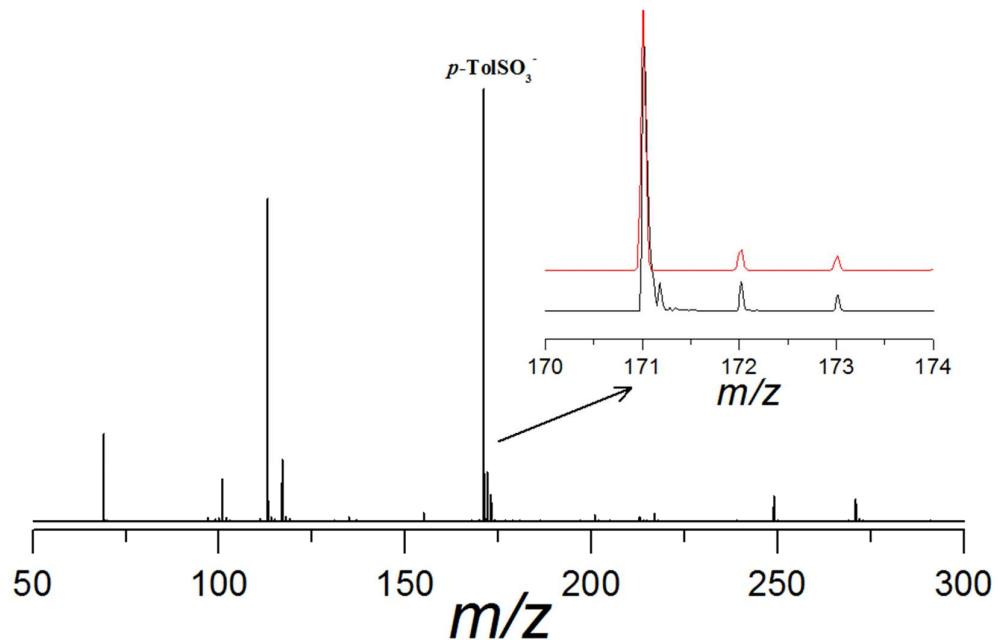


Figure S10: The compared Adsorption Capacity for selective adsorption dichromate anion.

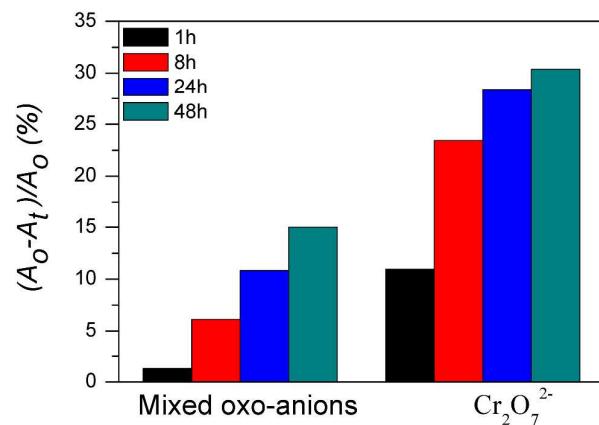


Figure S11: The energy dispersive spectroscopy (EDS) mapping of SD/Ag16.

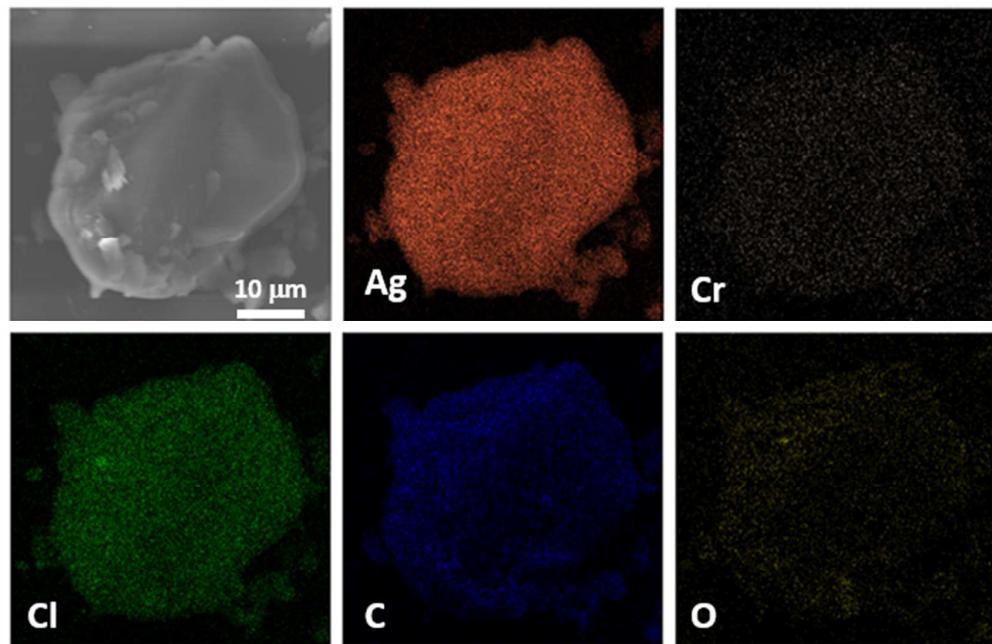
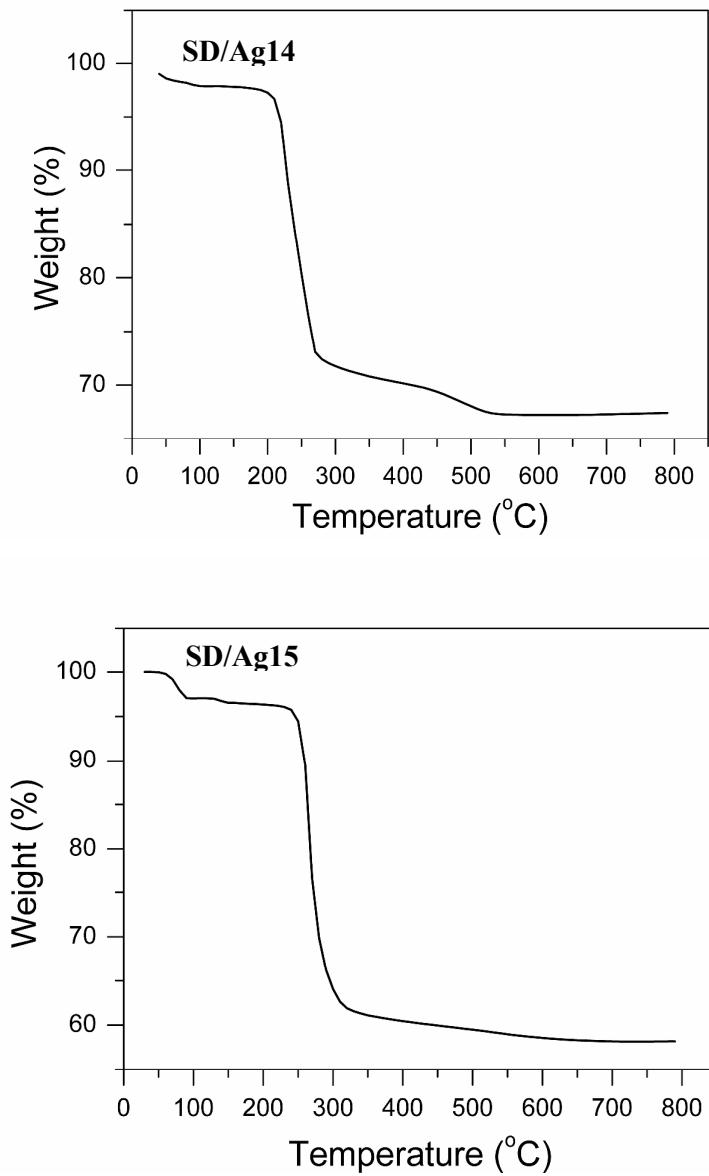


Figure S12: The TGA of SD/Ag14 and SD/Ag15.



Reference:

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