Electronic Supporting Information

Facile construction of an Ag⁰-doped Ag(I)-based coordination polymer *via* self-photoreduction strategy for enhanced visible light driven photocatalysis

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Experimental

Materials and characterization

All the chemical reagents were obtained commercially and used without further purification. The infrared (IR) spectrum was collected on a Nicolet iS50 FT-IR spectrometer (ThermoFisher, United States). Elemental analysis (C, H, N) was performed on a VarioEL III Elemental Analyzer (Elementar, Germany). The crystalline structures of the materials were analyzed by PXRD (Rigaku, Dmax 2000) with CuK α radiation ($\lambda = 1.5406$ Å) at room temperature in the range of 5°-80°. The morphology and size of samples were observed by SEM (Hitachi, Regulus 8100) a. The XPS characterizations were obtained on an ESCALAB250XI electron spectrometer (VG Scientific,

America). The UV-vis diffuse reflectance spectra (DRS) were collected by a UV-vis spectrophotometer (UV-2550, Shimidazu). Photocurrents and EIS were recorded using a PGSTAT-302N electrochemical workstation. The photoluminescence (PL) spectra were measured using a F4500 (Hitachi, Japan) photoluminescence detector with an excitation wavelength of 300 nm. ESR analyses were performed on the Bruker EPR JES-FA200 spectrometer.

Photoelectrochemical measurements

Photoelectrochemical performances of the prepared photo-anodes were recorded on an electrochemical work station (CHI760E) with a standard three electrode system. 0.5 M Na₂SO₄ solution was used as the electrolyte. A 300W Xe lamp (Beijing PerfectLight) was used as a light source. Transient photocurrent measurements at a constant bias (0.8 V) with chopped illumination were also conducted to examine the steady-state photocurrent densities of the photoanodes. Electrochemical impedance spectra (EIS) were carried out in the frequency range of 1-10⁵ Hz. The Mott-Schottky measurement was performed at the frequency of 1000 Hz.

X-ray crystallorgraphy

Crystal data was collected Bruker Smart Apex II CCD diffractometer with graphitemonochromatic MoK α radiation ($\lambda = 0.71073$ Å) at room temperature. The structures were solved by direct methods of *SHELXS-2014* and refined on F^2 by full-matrix least-squares using the *SHELXL-2014 within WINGX* [1,2]. All the calculations were performed under *WINGX* program. All non-hydrogen atoms were refined anisotropically, and the hydrogen atoms of organic ligands and water molecules were generated geometrically. The crystallographic data for **JLNU-90** is listed in Table S1, selected bond lengths and bond angles are summarized in Table S2.

Compound	JLNU-90
Empirical formula	$C_{32}H_{30}N_7O_{8.5}Ag_2$
Formula weight	864.37
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> (Å)	11.388(3)

Table S1 Selected crystallographic data for JLNU-90

<i>b</i> (Å)	12.621(3)
c (Å)	14.493(4)
α (°)	100.520(5)
β (°)	109.121(5)
γ (°)	97.132(5)
$V(Å^3)$	1896.8(8)
Z	2
Goodness-of-fit on F ²	0.589
Refins collected/unique	13005
θ Range (°)	3.06-51.3
$R (I > 2\sigma(I))$	$R_1 = 0.0531$,
	wR ₂ =0.1597
R (all data)	$R_1 = 0.1075$,
	wR ₂ =0.2046
CCDC	2079891

Table S2 Selected bond distances (Å) and angles (°) for JLNU-90.

Ag(1)-N(2) ^{#1}	2.140(5)	Ag(2)-N(3) ^{#1}	2.170(4)
Ag(1)-N(1)	2.159(4)	Ag(2)-N(4)	2.180(4)
Ag(1)-O(3)	2.262(4)	Ag(2)-O(4)	2.591(4)
N(2) ^{#1} -Ag(1)-N(1)	174.92(16)	N(3) ^{#1} -Ag(2)-N(4)	168.83(15)
N(2) ^{#1} -Ag(1)-O(3)	91.39	N(3)-Ag(2)-O(4)	95.30(18)
N(1)-Ag(1)-O(3)	93.66	N(4)-Ag(2)-O(4)	91.07(17)

Symmetry code: #1 1+x, y, z.



Fig. S1. TG curve of the as-synthesized JLNU-90.

The guest molecules in **JLNU-90** were evaluated through TG analysis (Fig. S1). The lost weight of before 100 °C corresponds to the release of wo acetonitrile and two and a half water molecules (obsd 18.15 %, calcd 17.23 %). The second weight loss occurs from 180 °C should be attributed to the decomposition of organic ligands.



Fig. S2. The optical photographs of JLNU-90 and JLNU-90/1.5.



Fig. S3. The XPS survey spectrum of JLNU-90/1.5.

Catalysts	Light source	MB concentration (mg/L)	Dosage of catalysts	Time (min)	Degradation efficiency (%)	k value (min ⁻¹)	Ref.
JLNU-90/1.5	10 W LED (vis)	10	20 mg	120	70	0.00896	This work
[Ag(HIPA)(L)] _n	500 W Hg lamp (UV)	10	0.01 mmol	150	95.9	0.0177	3
[Ag(L)(HNTP)] _n	500 W Hg lamp (UV)	10	0.01 mmol	240	93.5	0.0106	4
$[Ag_2(dmt)_2(tph)]_n$	300 W Hg lamp (UV)	3.2	100 mg	130	96	0.015	5
[Ag ₂ (dmt) ₂ (oxalate)] _n	300 W Hg lamp (UV)	3.2	100 mg	130	~80	0.011	5
$[\mathrm{Ag}_2(\mathrm{dmt})_4(\mathrm{SO}_4)]\cdot_2(\mathrm{dmt})\cdot_2(\mathrm{H}_2\mathrm{O})$	300 W Hg lamp (UV)	3.2	100 mg	130	~68	0.007	5
$[Ag_4(L^1)_2(HSiW^{VI}_{11}V^VO_{40})] \sim 25H_2O$	UV	6.4	150 mg	120	93	-	6
$[Ag_4(L^2)_2(H_2O)_2(PW^{VI}_{11}V^VO_{40})]\cdot 2H_2$ O	UV	6.4	150 mg	120	87.3	-	6

Table S3. Comparison of Ag(I)-based coordination polymers



Fig. S4. (a) UV-vis DRS and (b) direct energy band gap of JLNU-90 and JLNU-90/x.



Fig. S5. PL spectra of JLNU-90 and JLNU-90/x.



Fig. S6. The Mott-Schott curve of JLNU-90.

Reference

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