

Electronic supplementary information for:

Structure, photoluminescence emissions, and photocatalytic activity of Ag₂SeO₃: a joint experimental and theoretical investigation

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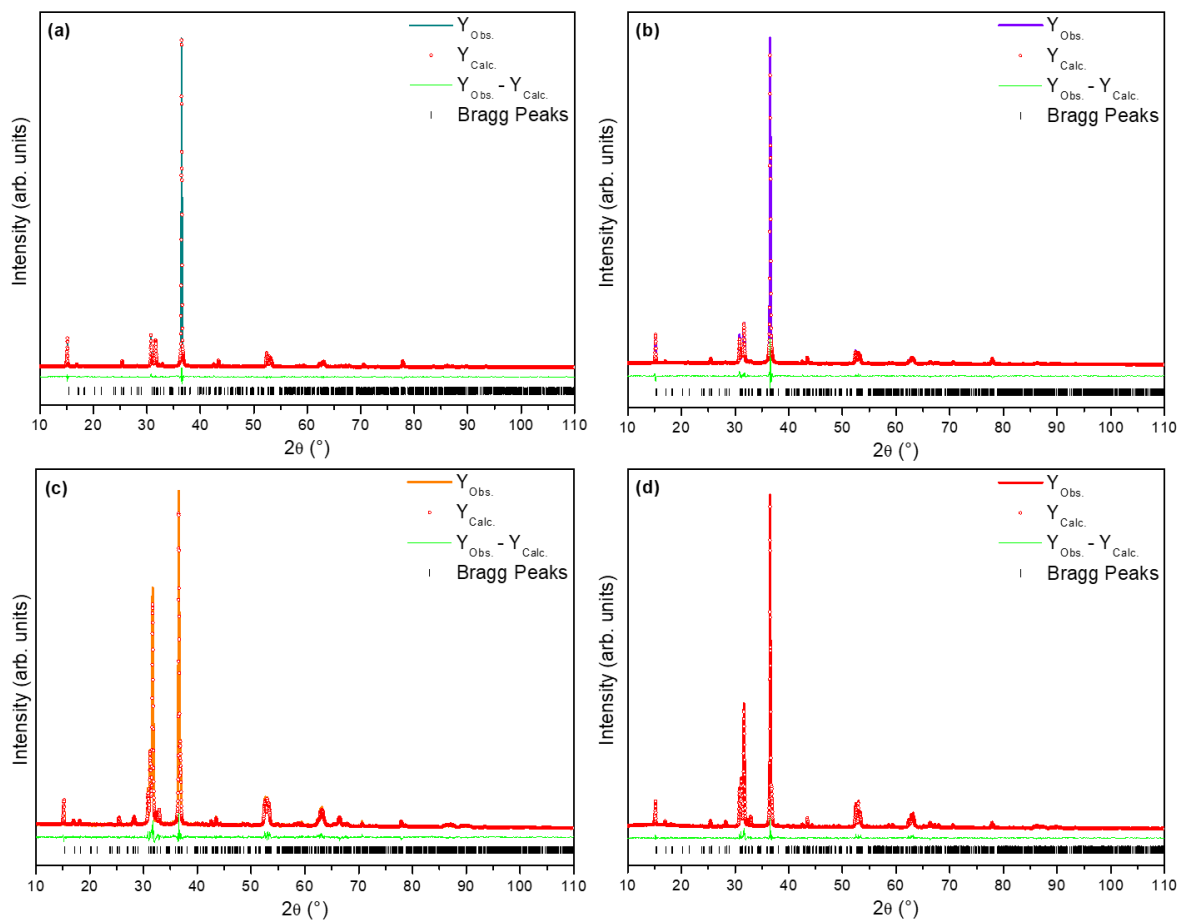


Figure SI-1. Rietveld refinement plot of (a) $\text{Ag}_2\text{SeO}_3\text{-SC}$, (b) $\text{Ag}_2\text{SeO}_3\text{-UP}$, (c) $\text{Ag}_2\text{SeO}_3\text{-CP}$ and (d) $\text{Ag}_2\text{SeO}_3\text{-MH}$ microcrystals.

Table SI-1. Atomic positions of the Ag₂SeO₃ microcrystals.

Atoms	Ag ₂ SeO ₃ -SC			Ag ₂ SeO ₃ -UP		
	x	y	z	x	y	z
Ag1	0.2708(7)	0.2528(6)	0.0891(8)	0.2616(0)	0.2519(0)	0.0916(0)
Ag2	0.2519(2)	0.5862(1)	0.6366(1)	0.2526(0)	0.5837(0)	0.6357(0)
Se1	0.7394(8)	0.4066(6)	0.8335(4)	0.7398(0)	0.4083(0)	0.8358(0)
O1	0.4101(1)	0.3940(7)	0.8476(3)	0.3891(0)	0.3948(0)	0.8505(0)
O2	0.7696(4)	0.5366(8)	0.6878(1)	0.7623(0)	0.5371(0)	0.6864(0)
O3	0.8142(4)	0.2782(6)	0.6686(1)	0.7965(0)	0.2871(0)	0.6770(0)

Atoms	Ag ₂ SeO ₃ -CP			Ag ₂ SeO ₃ -MH		
	x	y	z	x	y	z
Ag1	0.2616(0)	0.2519(0)	0.0916(0)	0.2598(2)	0.2538(0)	0.0893(6)
Ag2	0.2526(0)	0.5837(0)	0.6357(0)	0.2534(9)	0.5847(1)	0.6367(9)
Se1	0.7398(0)	0.4083(0)	0.8358(0)	0.7306(9)	0.4093(5)	0.8338(0)
O1	0.3891(0)	0.3948(0)	0.8505(0)	0.4024(8)	0.3897(3)	0.8477(6)
O2	0.7623(0)	0.5371(0)	0.6864(0)	0.8402(6)	0.5392(7)	0.7058(1)
O3	0.7965(0)	0.2871(0)	0.6770(0)	0.8079(0)	0.2973(7)	0.6624(9)

ICSD N°78388 Ag1 (x) 0.2616(2), (y) 0.2519(1), (z) 0.0916(2); Ag2 (x) 0.2526(2), (y) 0.5837(1), (z) 0.6357(1); Se1 (x) 0.7398(3), (y) 0.4083(1), (z) 0.8358(2); O1 (x) 0.3891(19), (y) 0.3948(8), (z) 0.8505(1); O2 (x) 0.7623(2), (y) 0.5371(9), (z) 0.6864(1); O3 (x) 0.7965(2), (y) 0.2871(8), (z) 0.6770(1)

Table SI-2. Crystallographic data of Rietveld refinement.

Parameters	Samples			
	Ag ₂ SeO ₃ -SC	Ag ₂ SeO ₃ -UP	Ag ₂ SeO ₃ -CP	Ag ₂ SeO ₃ -MH
Source	Cu K α	Cu K α	Cu K α	Cu K α
Chemical formula	Ag ₂ SeO ₃	Ag ₂ SeO ₃	Ag ₂ SeO ₃	Ag ₂ SeO ₃
Formula weight	342.69	342.69	342.69	342.69
Temperature	ambient	ambient	ambient	ambient
Pressure	ambient	ambient	ambient	ambient
Wavelength (Å)	1.5406	1.5406	1.5406	1.5406
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group (No.)	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P2₁/c</i>
<i>a</i> (Å)	4.8580(4)	4.8601(4)	4.85710(14)	4.85999(14)
<i>b</i> (Å)	10.33829(11)	10.33457(16)	10.33995(22)	10.33953(14)
<i>c</i> (Å)	6.95715(7)	6.95925(11)	6.95691(15)	6.95652(10)
α (°)	90.0	90.0	90.0	90.0
β (°)	91.085(4)	90.919(8)	90.9292(34)	91.1142(28)
γ (°)	90.0	90.0	90.0	90.0
<i>V</i> (Å ³)	349.348(27)	349.496(33)	349.345(15)	349.499(12)
<i>Z</i>	4	4	4	4
<i>d</i> -space range (Å)	0.94-5.77	0.94-5.77	0.94-5.77	0.94-5.77
χ^2	1.55	1.50	1.33	1.26
<i>R_p</i> (%)	7.93	9.76	9.82	8.59
<i>R_{wp}</i> (%)	12.53	13.75	13.90	11.90

R_p = profile *R*-factor; *R_{wp}* = weighted profile *R*-factor

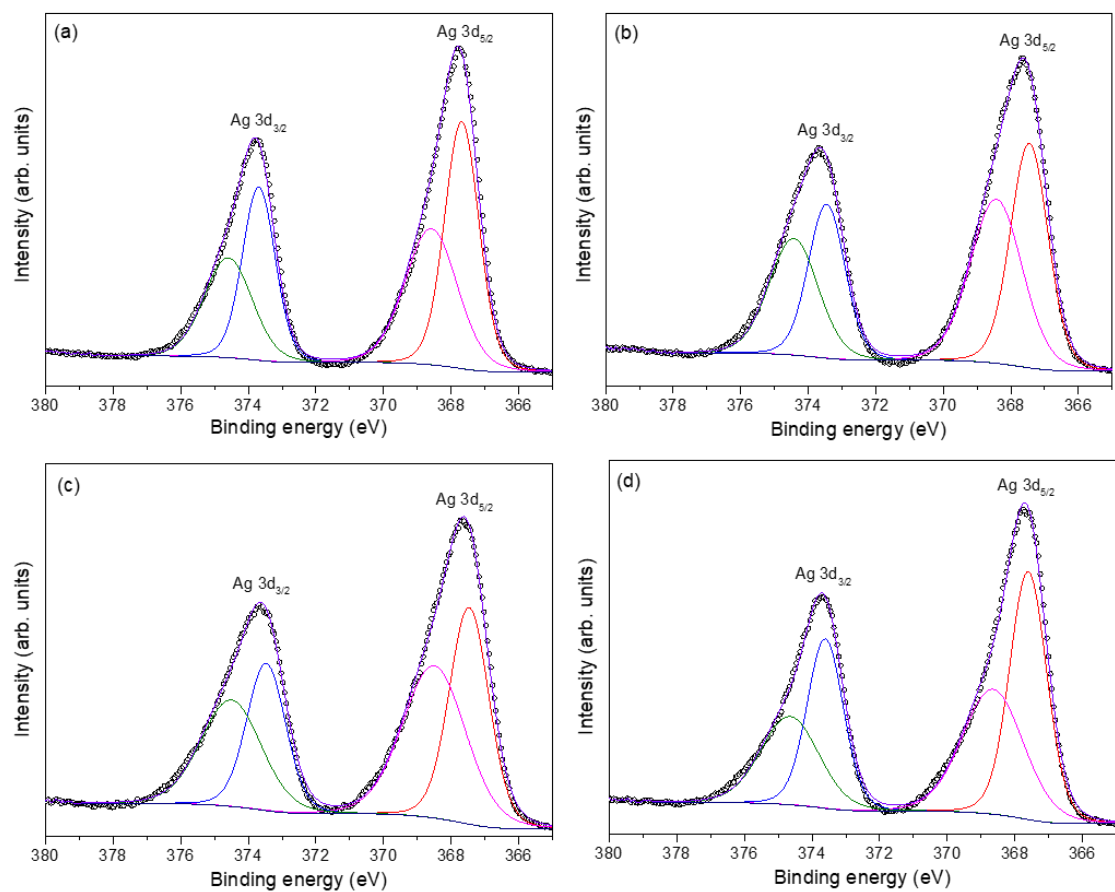


Fig. SI-2. Core level spectra of Ag 3d of the (a) $\text{Ag}_2\text{SeO}_3\text{-SC}$, (b) $\text{Ag}_2\text{SeO}_3\text{-UP}$, (c) $\text{Ag}_2\text{SeO}_3\text{-CP}$, and (d) $\text{Ag}_2\text{SeO}_3\text{-MH}$ samples.

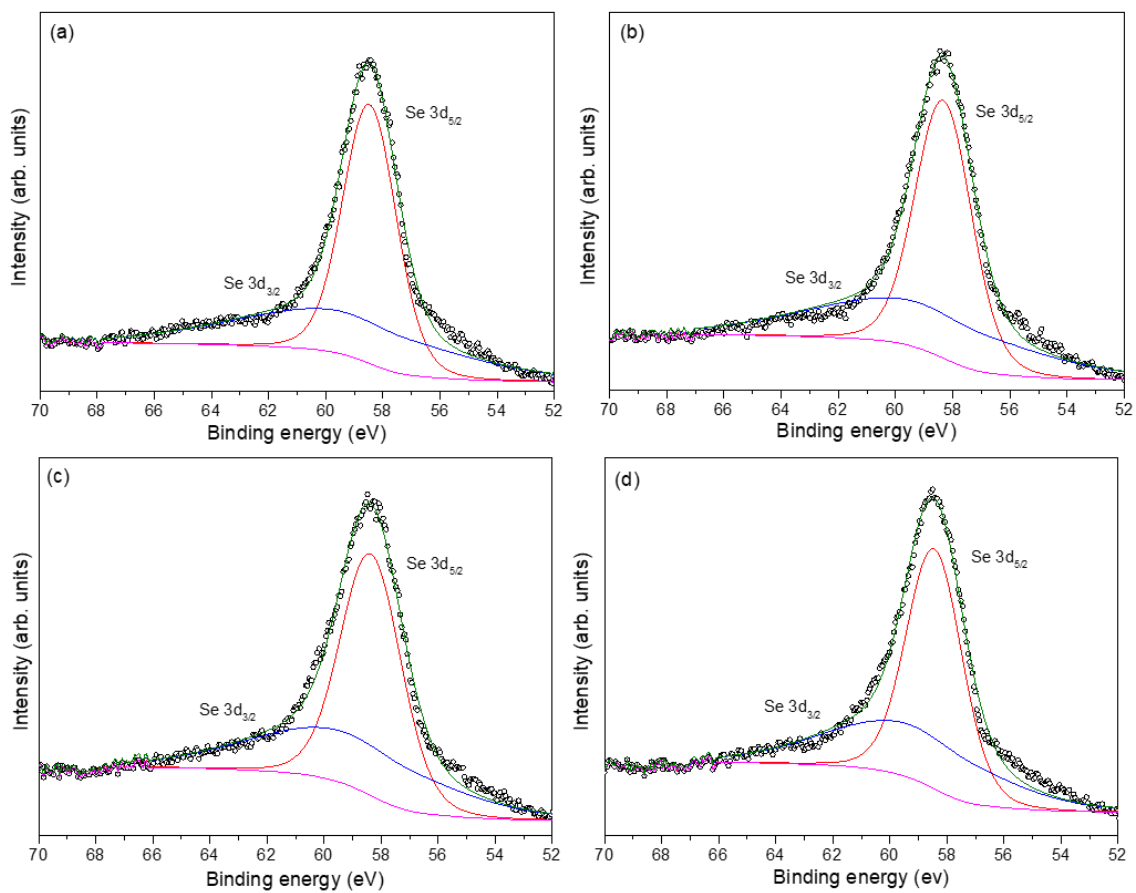


Fig. SI-3. Core level spectra of Se 3d of the (a) $\text{Ag}_2\text{SeO}_3\text{-SC}$, (b) $\text{Ag}_2\text{SeO}_3\text{-UP}$, (c) $\text{Ag}_2\text{SeO}_3\text{-CP}$, and (d) $\text{Ag}_2\text{SeO}_3\text{-MH}$ samples.

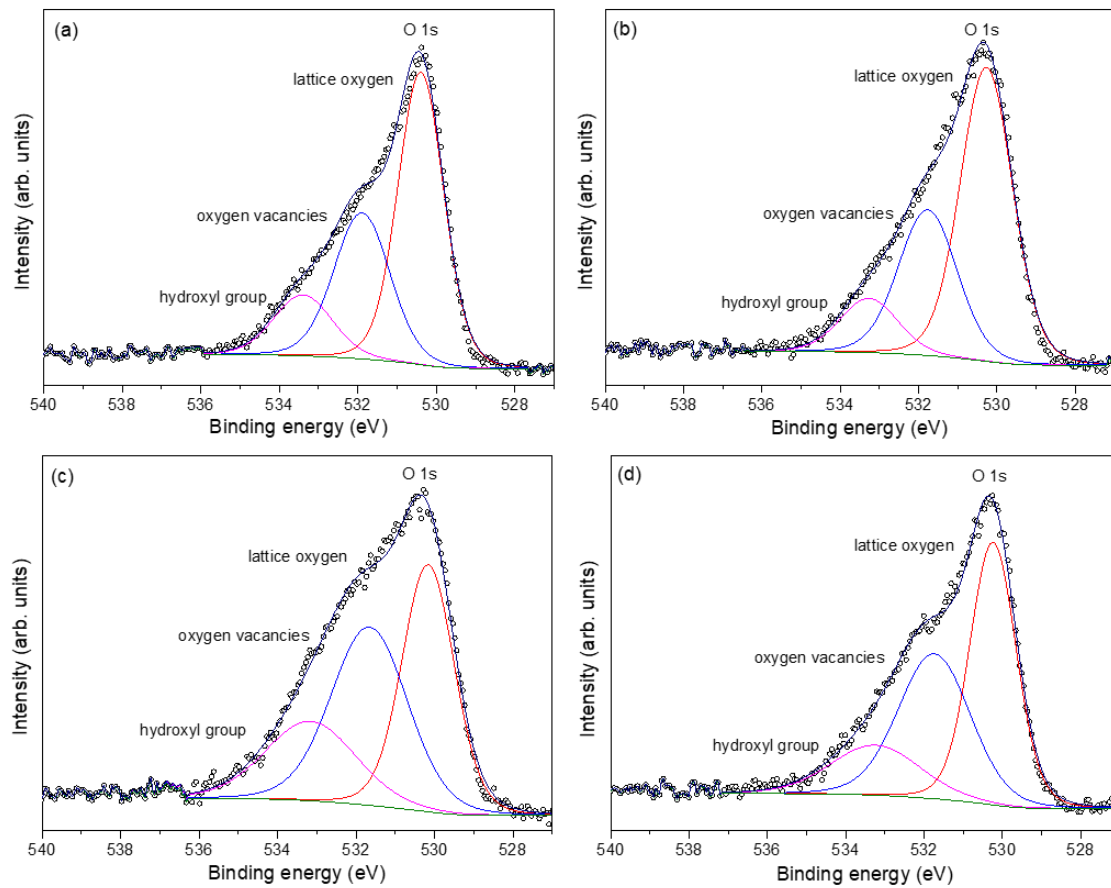


Fig. SI-4. Core level spectra of O 1s of the (a) $\text{Ag}_2\text{SeO}_3\text{-SC}$, (b) $\text{Ag}_2\text{SeO}_3\text{-UP}$, (c) $\text{Ag}_2\text{SeO}_3\text{-CP}$, and (d) $\text{Ag}_2\text{SeO}_3\text{-MH}$ samples.

Table SI-3. XPS elements positions and concentration of the area components for Ag, Se and O of the Ag_2SeO_3 samples.

Samples	Elements	Ag (3d)				Se (3d)		O (1s)		
	oxidation states	Ag^+		Ag^0		Se^{4+}		O^{2-}		
	spin-orbit components	$3d_{5/2}$	$3d_{3/2}$	$3d_{5/2}$	$3d_{3/2}$	$3d_{5/2}$	$3d_{3/2}$	Lattice oxygen	Oxygen vacancies	Hydroxyl group
Ag_2SeO_3 -SC	Position (eV)	367.7	373.7	368.6	374.6	58.47	59.33	530.4	531.9	533.4
	Conc. (%)	27.61	26.69	23.24	22.46	50.78	49.22	53.36	32.45	14.19
Ag_2SeO_3 -UP	Position (eV)	367.5	373.5	368.5	374.5	58.33	59.19	530.3	531.8	533.3
	Conc. (%)	25.29	24.45	25.55	24.70	50.62	49.38	56.93	31.47	11.60
Ag_2SeO_3 -CP	Position (eV)	367.5	373.5	368.5	374.5	58.36	59.22	530.2	531.7	533.2
	Conc. (%)	23.98	23.18	26.86	25.97	50.62	49.38	38.28	40.38	21.34
Ag_2SeO_3 -MH	Position (eV)	367.5	373.5	368.7	374.7	58.44	59.30	530.2	531.7	533.2
	Conc. (%)	27.78	26.85	23.07	22.30	50.62	49.38	44.91	38.55	16.53

Table SI-4. Surface area composition, E_{surf} and E_{poly} for the different proposed morphologies.

Surface	E_{surf} (% C_i)						
	Ideal	A1	A2	A3	B1	B2	B3
(011)	0.23(67.2)	0.70 (0.0)	0.70 (0.00)	1.10 (0.00)	0.23(58.4)	0.23(40.6)	0.23(41.4)
(100)	0.25(31.5)	0.25(45.0)	0.25(38.7)	0.25(35.1)	0.25(32.4)	0.51(9.02)	0.51(11.4)
(001)	0.30(0.00)	0.30(37.5)	0.15(54.5)	0.15(58.6)	0.30(0.00)	0.30(0.00)	0.30(0.00)
(021)	0.35(0.00)	2.20(0.0)	2.20(0.00)	2.20(0.00)	0.30(9.24)	0.25(18.1)	0.23(29.3)
(110)	0.36(1.23)	2.20(0.0)	2.20(0.00)	2.20(0.00)	0.36(1.23)	0.51(7.81)	0.51(8.57)
(111)	0.37(0.00)	2.20(0.0)	2.20(0.00)	2.20(0.00)	0.51(0.00)	0.51(3.15)	0.80(0.00)
(010)	0.64(0.00)	0.64(17.5)	0.64(12.8)	1.40(6.28)	0.64(0.00)	0.23(21.3)	0.23(9.23)
(101)	0.70(0.00)	0.7(0.0)	2.0(0.00)	2.0(0.00)	0.70(0.00)	0.70(0.00)	0.70(0.00)
E_{poly}	0.24	0.34	0.25	0.26	0.24	0.29	0.27

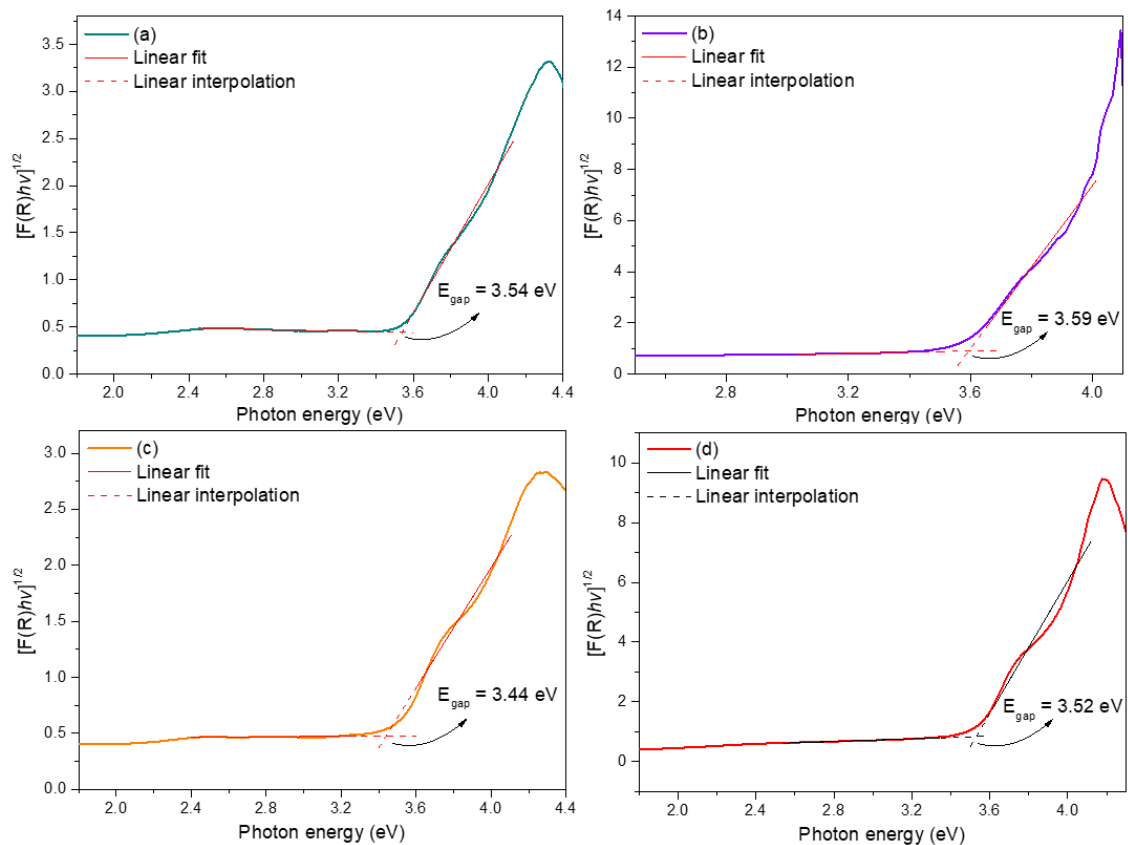


Fig. SI-5. Band gap energy estimated by Kubelka and Munk for the (a) $\text{Ag}_2\text{SeO}_3\text{-SC}$, (b) $\text{Ag}_2\text{SeO}_3\text{-UP}$, (c) $\text{Ag}_2\text{SeO}_3\text{-CP}$, and (d) $\text{Ag}_2\text{SeO}_3\text{-MH}$ samples.

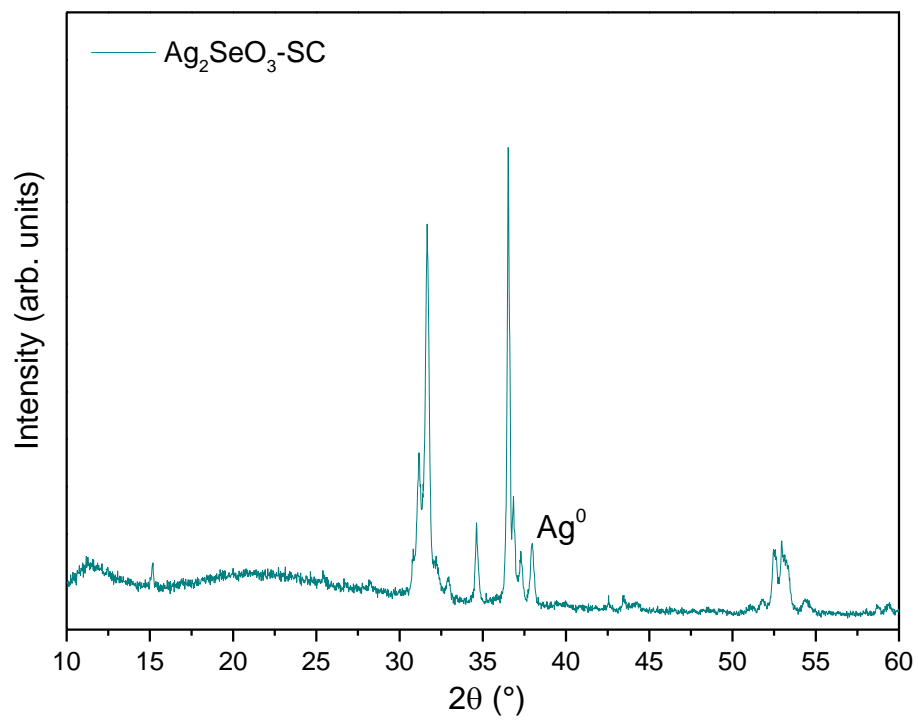


Fig. SI-6. XRD patterns of the Ag₂SeO₃-SC catalysts after 3 photocatalytic cycles.