Electronic supplementary information for:

Towards a relationship between photoluminescence emissions and photocatalytic activity of Ag_2SeO_4: Combining experimental data and theoretical insights

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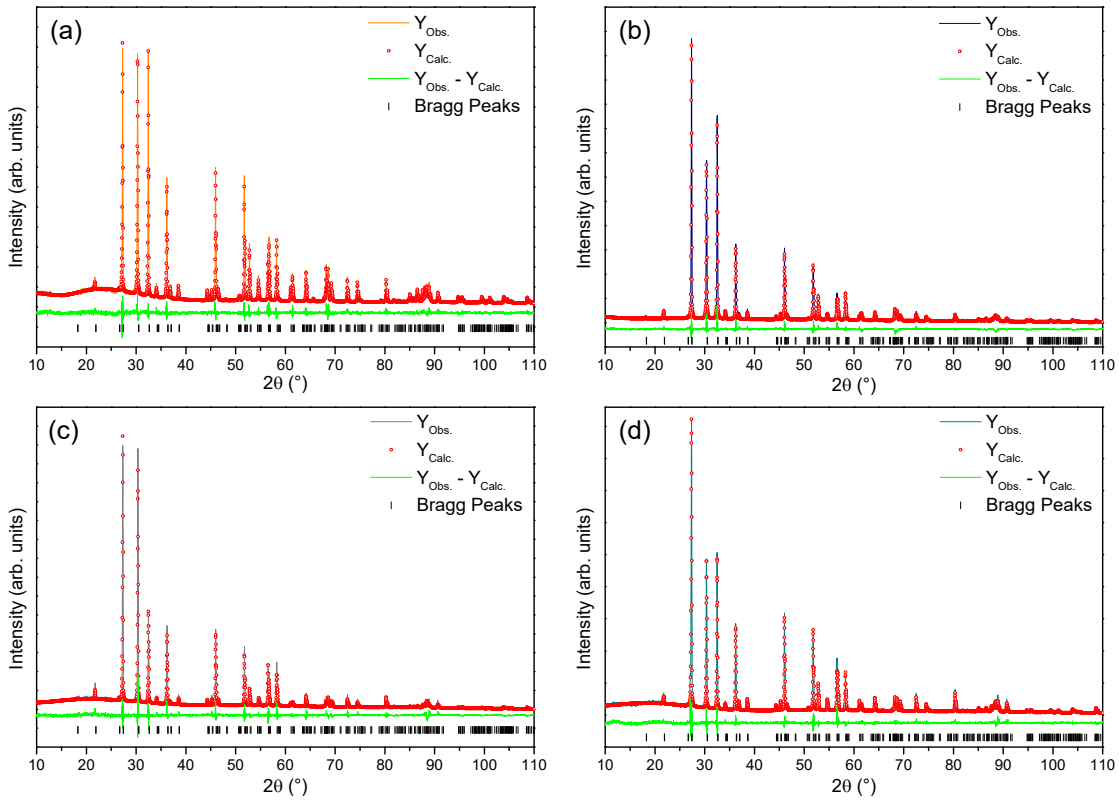

Figure SI-1. Rietveld refinement plot of (a) Ag_2SeO_4-SC, (b) Ag_2SeO_4-UP, (c) Ag_2SeO_4-CP and (d) Ag_2SeO_4-MH microcrystals.

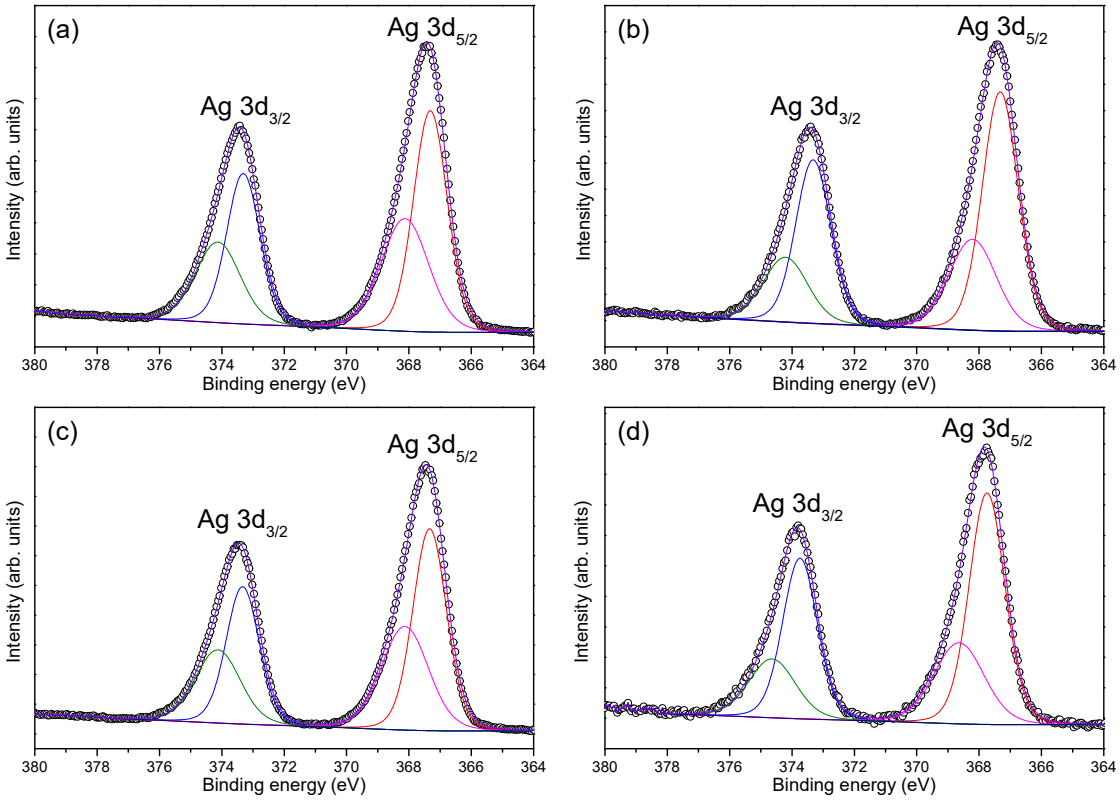

Figure SI-2. Core level spectra of Ag 3d of the (a) Ag_2SeO_4-SC, (b) Ag_2SeO_4-UP, (c) Ag_2SeO_4-CP, and (d) Ag_2SeO_4-MH samples.

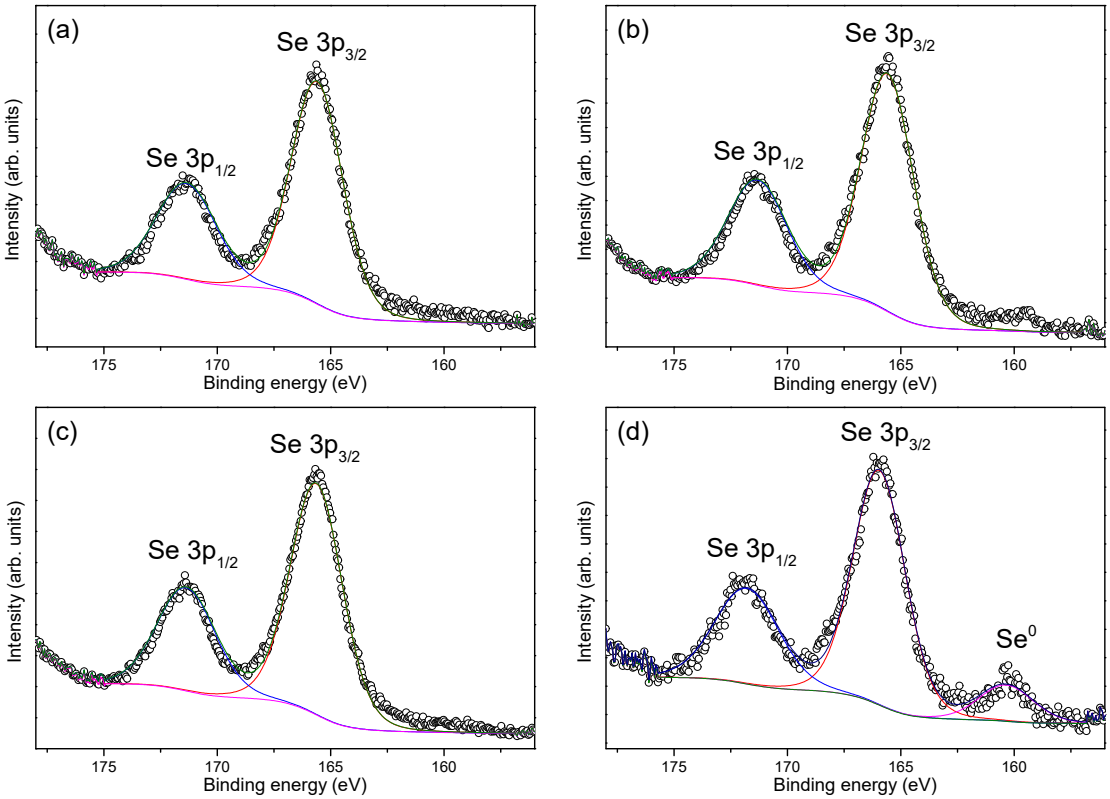

Figure SI-3. Core level spectra of Se 3p of the (a) Ag_2SeO_4-SC, (b) Ag_2SeO_4-UP, (c) Ag_2SeO_4-CP, and (d) Ag_2SeO_4-MH samples.

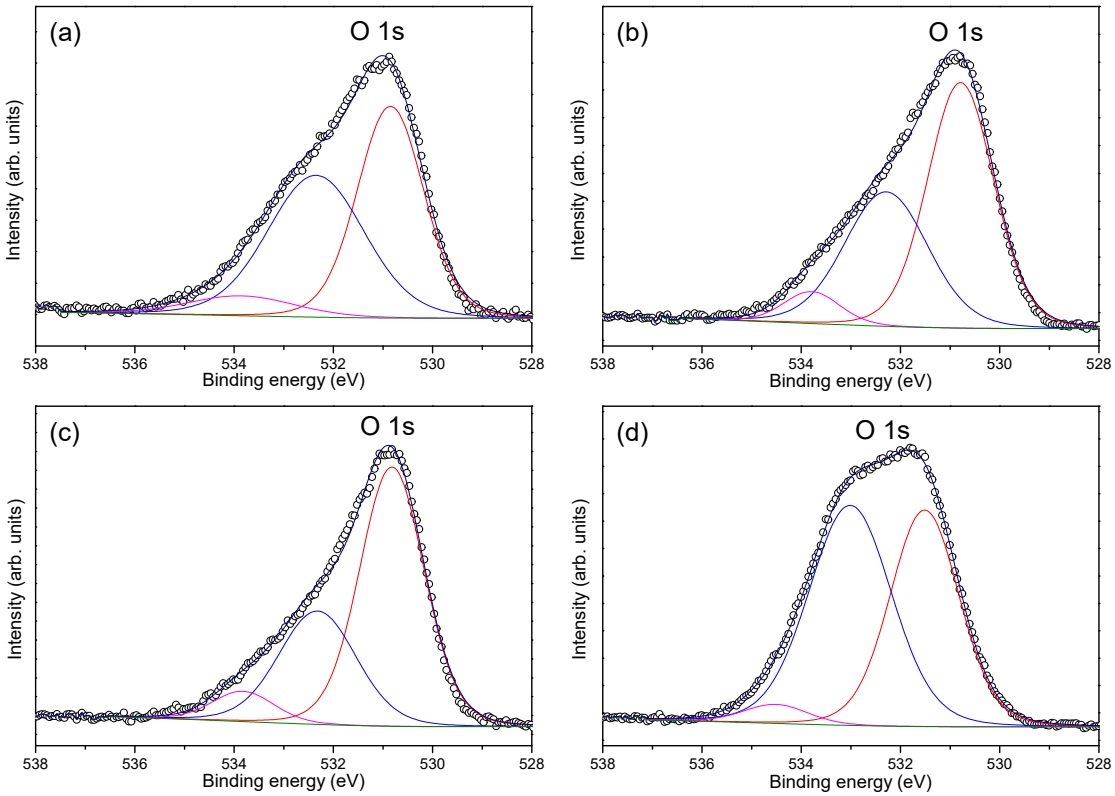

Figure SI-4. Core level spectra of O 1s of the (a) Ag_2SeO_4-SC, (b) Ag_2SeO_4-UP, (c) Ag_2SeO_4-CP, and (d) Ag_2SeO_4-MH samples.

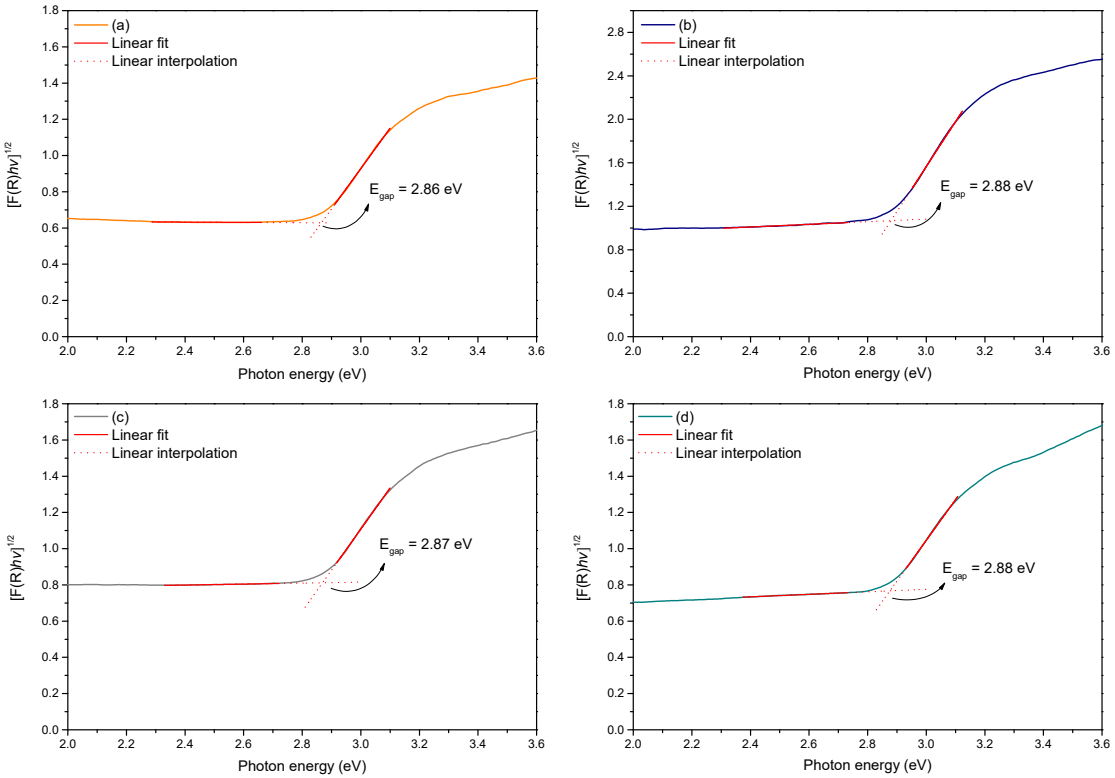

Figure SI-5. Band gap energy for the (a) Ag_2SeO_4-SC, (b) Ag_2SeO_4-UP, (c) Ag_2SeO_4-CP, and (d) Ag_2SeO_4-MH samples.

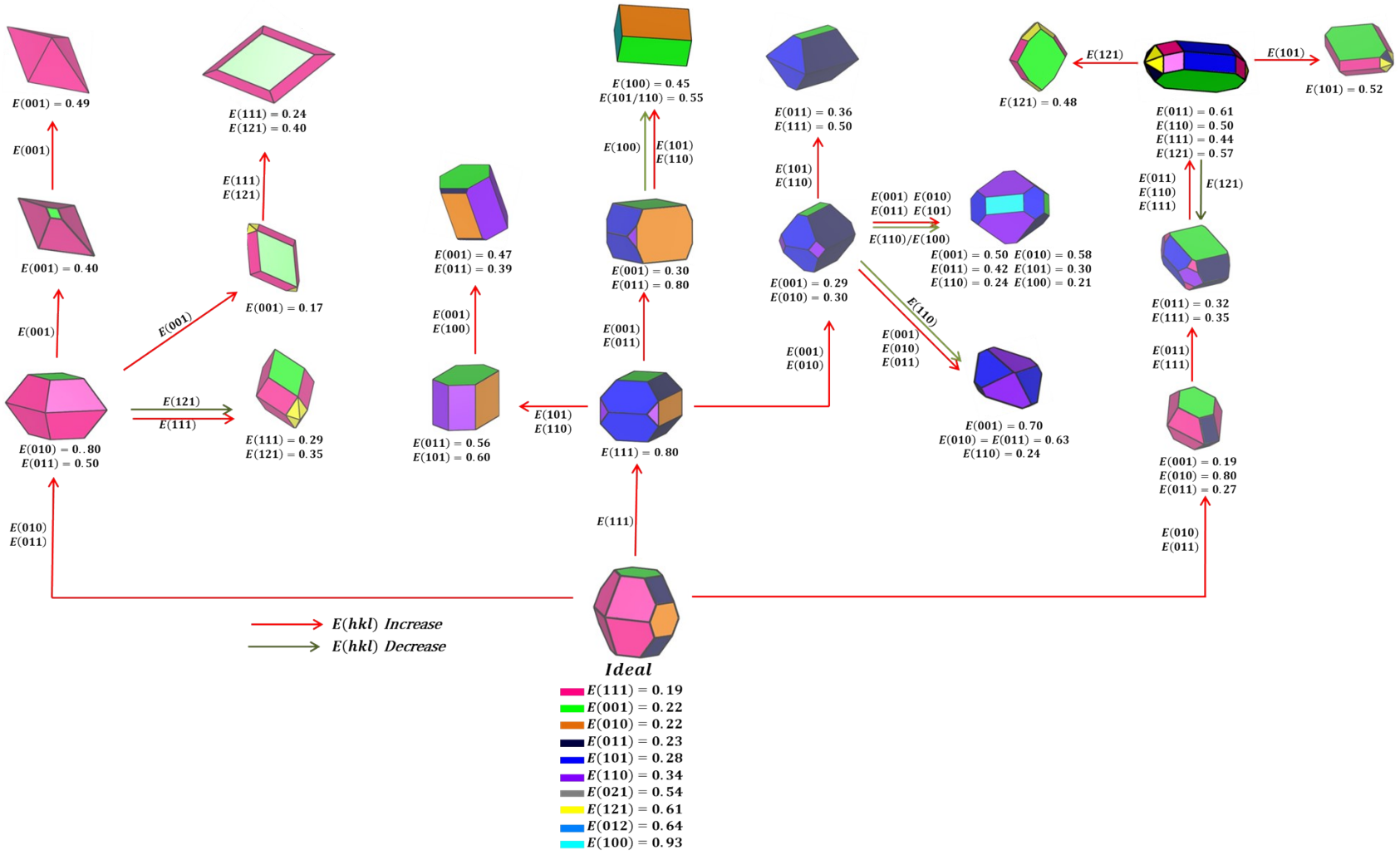

Figure SI-6. Crystals shape theoretically modeled by the Wulff construction and their energy relative surface for Ag_2SeO_4. *E(hkl)* in Jm^{-2}.

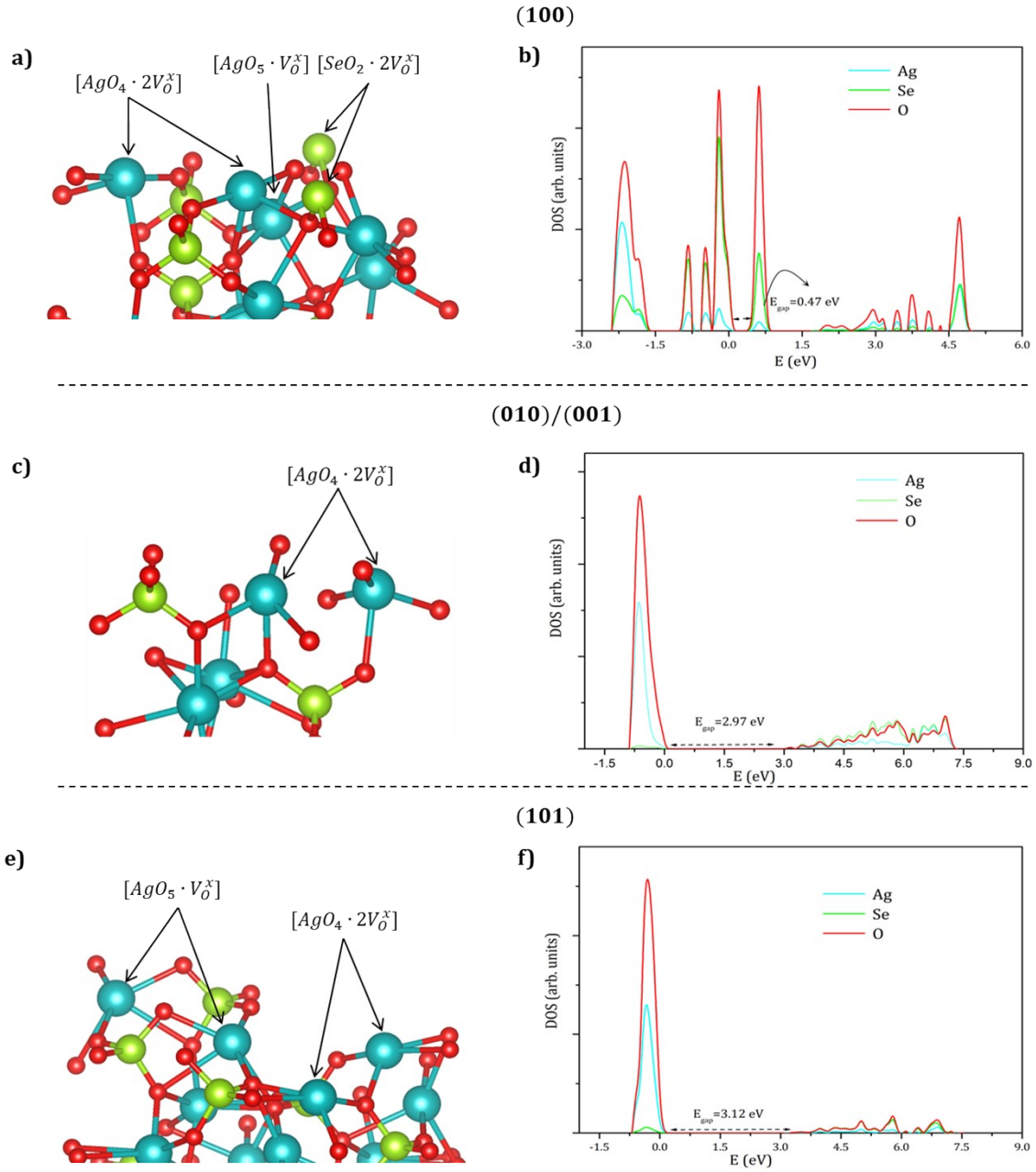

Figure SI-7. Geometric structure and DOS of surface atoms in the relaxed surface slab: (a-b) (100) surface, (c-d) (010)/001 surfaces, and (e-f) (101) surface

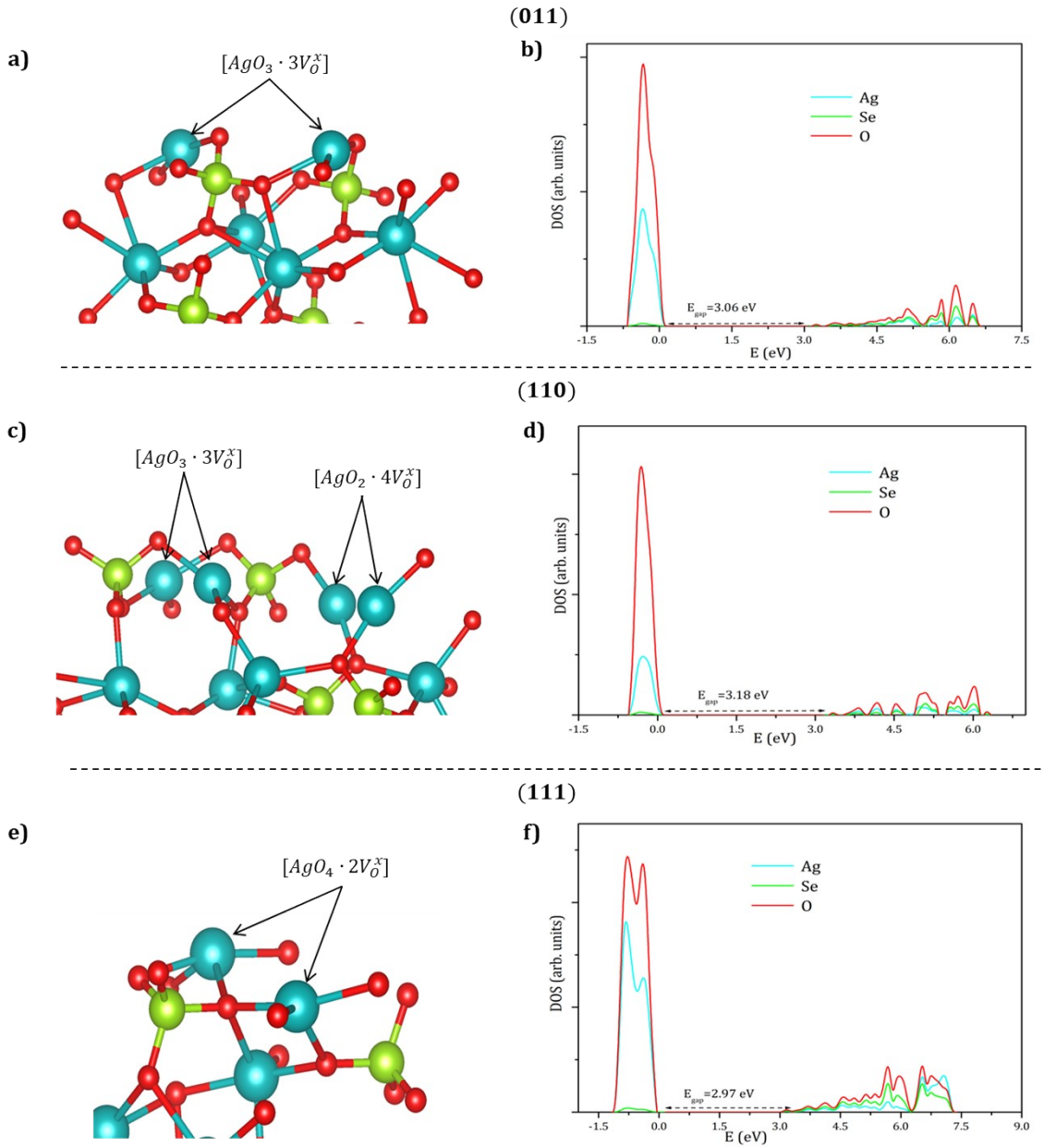

Figure SI-8. Geometric structure and DOS of surface atoms in the relaxed surface slab: (a-b) (011) surface, (c-d) (110) surface, and (e-f) (111) surface

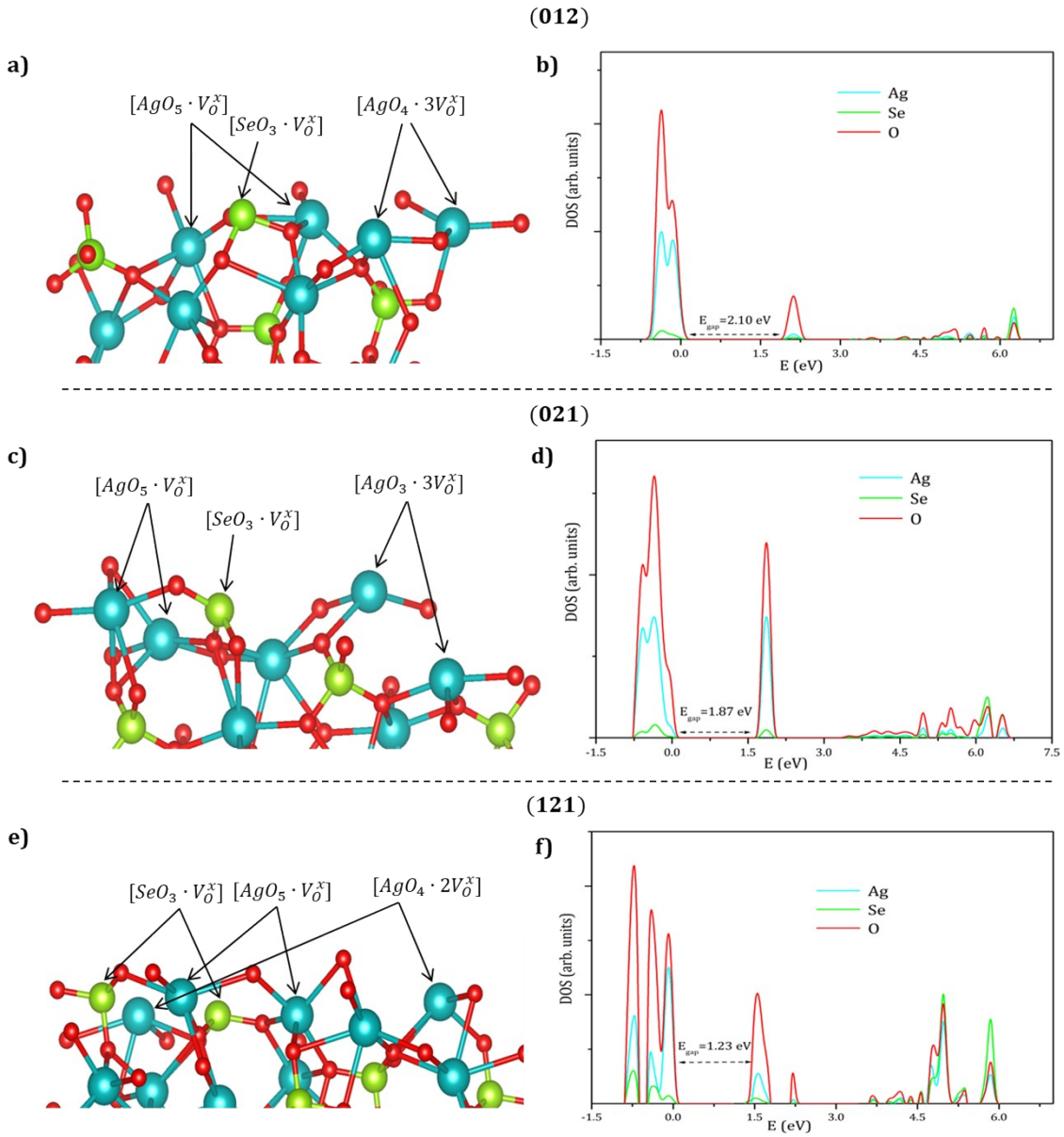

Figure SI-9. Geometric structure and DOS of surface atoms in the relaxed surface slab: (a-b) (012) surface, (c-d) (021) surface, and (e-f) (121) surface

Table SI-1. 2D lattice parameters of surface primitive cell, Area of surface in nm^2, number of bulk units (n) used in the slab construction and number of layers in the optimized slab.

Surface	2D Lattice parameter	*Area*	*n*	*layers*
(100)	$a = 8.483$ A $b = 8.062$ A $\gamma = 95.247°$	0.709	4	24
(010)	$a = 6.190$ A $b = 7.057$ A $\gamma = 116.014°$	0.393	3.5	35
(001)	$a = 6.039$ A $b = 6.089$ A $\gamma = 119.731°$	0.335	3.5	21
(101)	$a = 7.041$ A $b = 11.146$ A $\gamma = 90°$	0.784	5	25
(011)	$a = 6.076$ A $b = 8.678$ A $\gamma = 90°$	0.521	4	28
(110)	$a = 6.522$ A $b = 12.543$ A $\gamma = 90°$	0.813	6	42
(111)	$a = 6.219$ A $b = 7.112$ A $\gamma = 100.722°$	0.440	3	42
(012)	$a = 6.057$ A $b = 12.851$ A $\gamma = 103.887°$	0.780	5	70
(021)	$a = 6.198$ A $b = 13.802$ A $\gamma = 99.904°$	0.864	4	56
(121)	$a = 6.819$ A $b = 15.477$ A $\gamma = 95.345°$	0.112	5	55

Table SI-2. Atomic positions of the Ag_2SeO_4 microcrystals.

Atoms	Ag_2SeO_4-SC			Ag_2SeO_4-UP		
	x	y	z	x	y	z
Ag1	0.1250	0.4475	0.1250	0.1250	0.4475	0.1250
Se1	0.1250	0.1250	0.1250	0.1250	0.1250	0.1250
O1	0.2725	0.0281	0.0468	0.2995	0.0321	0.0416

Atoms	Ag_2SeO_4-CP			Ag_2SeO_4-MH		
	x	y	z	x	y	z
Ag1	0.1250	0.4475	0.1250	0.1250	0.4475	0.1250
Se1	0.1250	0.1250	0.1250	0.1250	0.1250	0.1250
O1	0.2450	0.0652	0.0196	0.2634	0.0251	0.0413

Table SI-3. Crystallographic data of Rietveld refinement.

Parameters	Samples			
	Ag_2SeO_4-SC	**Ag_2SeO_4-UP**	**Ag_2SeO_4-CP**	**Ag_2SeO_4-MH**
Source	Cu Kα	Cu Kα	Cu Kα	Cu Kα
Chemical formula	Ag_2SeO_4	Ag_2SeO_4	Ag_2SeO_4	Ag_2SeO_4
Formula weight	358.69	358.69	358.69	358.69
Temperature	ambient	ambient	ambient	ambient
Pressure	ambient	ambient	ambient	ambient
Wavelength (Å)	1.5406	1.5406	1.5406	1.5406
Crystal system	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space group (No.)	*Fddd*	*Fddd*	*Fddd*	*Fddd*
***a* (Å)**	6.05142(7)	6.05279(10)	6.05335(17)	6.05196(10)
***b* (Å)**	10.39899(16)	10.40138(24)	10.39740(25)	10.39745(23)
***c* (Å)**	12.98369(11)	12.98497(16)	12.98864(18)	12.98219(13)
***α* (°)**	90.0	90.0	90.0	90.0
***β* (°)**	90.0	90.0	90.0	90.0
***γ* (°)**	90.0	90.0	90.0	90.0
***V* (Å^3)**	817.047(16)	817.499(26)	817.493(32)	816.903(24)
Z	8	8	8	8
***d*-space range (Å)**	0.94-5.77	0.94-5.77	0.94-5.77	0.94-5.77
χ^2	1.22	1.34	1.35	1.27
R_p (%)	7.68	9.62	10.95	8.62
R_{wp} (%)	10.33	13.34	14.98	11.37

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

Table SI-4. XPS elements positions and concentration of the area components for Ag, Se and O of the Ag_2SeO_4 samples.

Samples	Elements	Ag 3d				Se 3p			O 1s		
	oxidation states	Ag^+		Ag^0		Se^{6+}		Se^0	O^{2-}		
	spin-orbit components	$3d_{5/2}$	$3d_{3/2}$	$3d_{5/2}$	$3d_{3/2}$	$3p_{3/2}$	$3p_{1/2}$	3p	Lattice oxygen	Oxygen vacancies	Hydroxyl group
Ag_2SeO_4-SC	**Position (eV)**	367.3	373.3	368.1	374.1	165.6	171.3	-	530.8	532.3	533.8
	Conc. (%)	29.64	28.65	21.21	20.50	51.02	48.98	-	47.03	45.88	7.09
Ag_2SeO_4-UP	**Position (eV)**	367.3	373.3	368.2	374.2	165.6	171.3	-	530.8	532.3	533.8
	Conc. (%)	33.95	32.81	16.90	16.34	51.02	48.98	-	55.60	38.30	6.10
Ag_2SeO_4-CP	**Position (eV)**	367.3	373.3	368.1	374.1	165.6	171.3	-	530.8	532.3	533.8
	Conc. (%)	29.61	28.62	21.24	20.53	51.02	48.98	-	61.14	32.04	6.82
Ag_2SeO_4-MH	**Position (eV)**	367.7	373.7	368.6	374.6	165.9	171.8	160.3	531.5	533.0	534.5
	Conc. (%)	34.12	32.98	16.73	16.17	48.40	46.47	5.12	43.52	52.94	3.54

Table SI-5. Surface energy (E_{surf}, Jm^{-2}), contribution of the surface area to the total area (C_i, %), and the polyhedron energy (E_{poly}, Jm^{-2}) for each of the crystal morphology of Ag_2SeO_4 obtained by SC, UP, CP and MH method.

Morphologies	**Ideal**		**A**		**B**		**C**		**D**		**E**		**F**		**G**	
Surface	E_{surf}	C_i	E_{surf}	C_i	E_{surf}	C_i	E_{surf}	C_i	E_{surf}	C_i	E_{surf}	C_i	E_{surf}	C_i	E_{surf}	C_i
(100)	0.93	-	0.93	-	0.93	-	0.93	-	0.93	-	0.40	21.71	0.93	-	0.93	-
(010)	0.22	9.84	0.41	-	0.80	-	0.80	-	0.80	-	0.22	44.40	0.80	-	0.80	-
(001)	0.22	14.29	0.46	-	0.17	34.72	0.17	39.98	0.22	29.04	0.30	32.56	0.19	41.94	0.19	48.62
(101)	0.28	-	0.28	-	0.28	-	0.50	-	0.50	-	0.55	-	0.28	28.99	0.52	-
(011)	0.23	12.84	0.32	-	0.50	-	0.50	-	0.50	-	0.80	-	0.61	3.98	0.61	3.30
(110)	0.34	-	0.37	-	0.34	-	0.34	-	0.34	-	0.55	-	0.50	-	0.50	-
(111)	0.19	63.07	0.19	100.0	0.24	67.44	0.27	59.43	0.29	65.29	0.80	-	0.44	17.14	0.44	41.47
(012)	0.64	-	0.64	-	0.64	-	0.64	-	0.64	-	0.64	-	0.64	-	0.64	-
(021)	0.54	-	0.54	-	0.54	-	0.54	-	0.54	-	0.54	-	0.80	-	0.80	-
(121)	0.61	-	0.61	-	0.61	-	0.40	0.06	0.35	5.67	0.61	-	0.57	7.95	0.57	6.61
E_{poly}	0.20		0.19		0.21		0.24		0.24		0.29		0.31		0.33	