

Supporting Information

Room Temperature Chemical Transformation of SnSe to Ag₂Se Nanocrystals via Cation Exchange[†]

Yiqiao Huang, Pierre F. P. Poudeu*

Table S1: Quantitative EDX analysis of Ag, Sn, and Se elements in SnSe precursor and Ag₂Se/SnSe nanocomposites

Sample code	Theoretical Ag at%	Experimental Ag at%	Theoretical Sn at%	Experimental Sn at%	Theoretical Se at%	Experimental Se at%
SnSe	0.0	0.000	50.0	47.7(2)	50.00	52.3(2)
A-10	9.5	9.6(1)	42.9	42.2(1)	47.6	48.1(2)
A-18	17.1	16.0(1)	37.1	33.6(1)	45.7	50.4(2)
A-20	18.2	17.7(1)	36.4	31.3(2)	45.5	51.0(2)
A-37	31.6	31.0(2)	26.4	22.9(2)	42.1	46.2(1)
A-50	40.0	38.6(2)	20.0	14.7(1)	40.0	46.7(2)
A-75	54.6	56.7(2)	9.1	3.4(0.2)	36.4	39.9(2)
A-100	66.7	64.2(1)	0.0	0.2(0.1)	33.3	35.7(1)

Table S2: Lattice parameters of SnSe and Ag₂Se, and phase composition of various SnSe/Ag₂Se nanocomposites extracted for the refinement of XRD data.

		SnSe	A-10	A-18	A-20	A-37	A-50	A-75	A-100
SnSe	a(Å)	11.518	11.522	11.522	11.524	11.529	11.526	11.657	-
	b(Å)	4.163	4.148	4.146	4.142	4.146	4.167	4.165	-
	c(Å)	4.409	4.440	4.453	4.454	4.448	4.418	4.411	-
	Unit cell volume(Å ³)	211.42	212.22	212.75	212.63	212.57	212.21	214.17	-
	Fraction of SnSe Nominal	100.0	90.0	81.3	80.0	62.5	50.0	25.0	0.0
	Fraction of SnSe Experimental	100.0	100.0	100.0	100.0	72.5(1)	40.5(2)	31.2(1)	0.0
	Bragg R-factor	8.8	2.6	2.7	2.1	2.4	5.0	4.9	-
Ag ₂ Se	a(Å)	-	-	-	-	4.329	4.331	4.338	4.331
	b(Å)	-	-	-	-	7.073	7.081	7.074	7.064
	c(Å)	-	-	-	-	7.807	7.831	7.789	7.777
	volume(Å ³)	-	-	-	-	239.05	240.19	239.01	237.95
	Fraction of Ag ₂ Se Nominal	0.000	10.000	18.750	20.000	37.500	50.000	75.000	100.000
	Fraction of Ag ₂ Se Experimental	0.000	0.000	0.000	0.000	27.5(1)	59.5(2)	68.8(1)	100.0
	Bragg R-factor	-	-	-	-	8.7	6.1	4.3	5.6

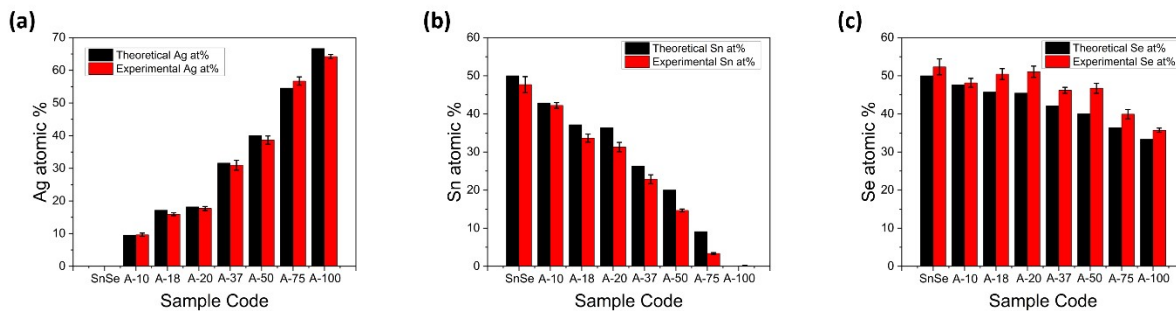


Figure S1: Quantitative EDX analysis showing the experimental and theoretical atomic percentages (a) Ag, (b) Sn, and (c) Se in various SnSe/Ag₂Se nanocomposites.

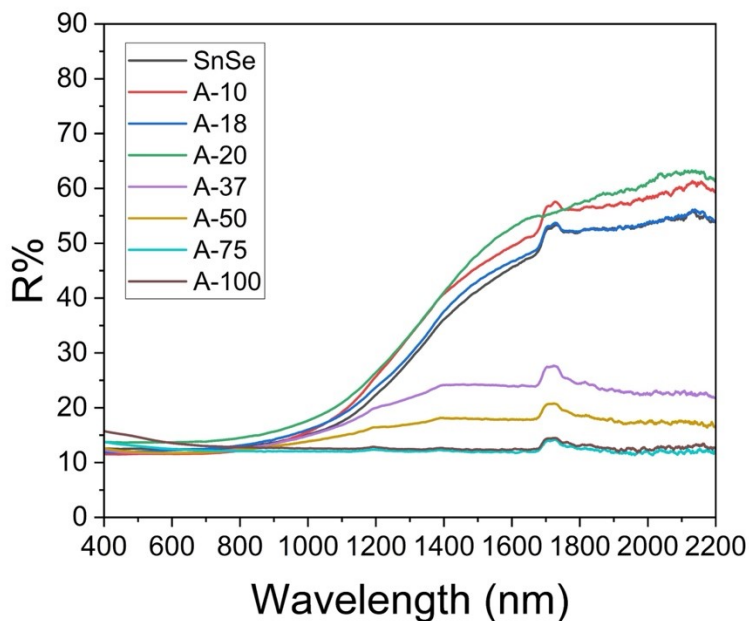


Figure S2: UV-Vis-NIR Diffuse reflectance data at 300 K on the SnSe precursor as well as on various SnSe/Ag₂Se nanocomposites.

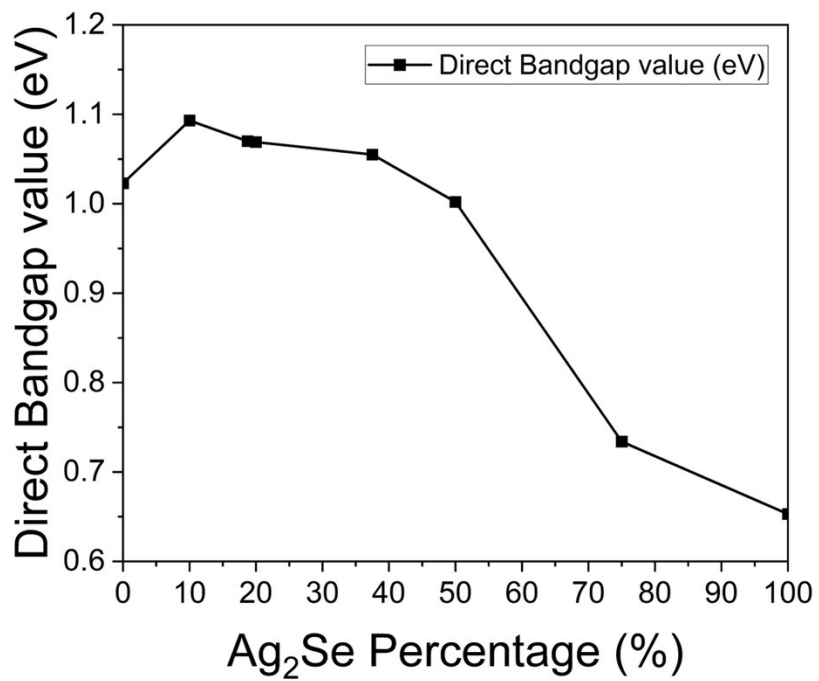


Figure S3: Change in band gap of various SnSe/Ag₂Se nanocomposites with increasing Ag₂Se content.