Supporting Information

Novel SnS_xSe_{1-x} Nanocrystals with Tunable Band Gap: Experimental and First-principles Calculations

Hao Wei,*[a] Yanjie Su,[a] Shangzhi Chen,[b] Yang Lin,[b] Zhi Yang,[a] Xiaoshuang Chen[c] and Yafei Zhang,*[a]

[a] Key Laboratory for Thin Film and Microfabrication of the Ministry of Education, Institute of Micro/Nano Science and Technology, Shanghai Jiao Tong University, Shanghai 200240, PR China. Tel.: +86 21 3420 5665; Fax: +86 21 3420 5665. E-mail address: haowei@sjtu.edu.cn (H. Wei), yfzhang@sjtu.edu.cn (Y. Zhang) .

b School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, PR China

[c] National Laboratory for Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, 200083 Shanghai, PR China

Experimental Section

I. Materials. Stannous oxide (SnO, >90.0%), selenium (Se, >99.95%), sulfur (S, >99.5%), octadecene (90%), oleic acid (OA, 90%), oleylamine (OLA, 70%) and trioctylphosphine (TOP, >97%) were purchased from Aladdin, without further purification.

II. Typical synthesis of SnS_xSe_{1-x} nanocrystals. 2 mmol SnO, 4 mL octadecene, and 5 mL OA were added to a 100 mL two-neck flask followed with vacuum pumping and N_2 bubbling. Then the solution was kept at 260 °C for 1 h. Meanwhile, TOP/Se solution, OLA/S solution were added to two 100 mL two-neck flask followed with vacuum pumping and N_2 bubbling. The Se and S ratio was tuned to different specific values, while the total amount was kept at 2 mmol. Then both solutions were kept at 60°C for 1 h. When the two solutions were completely dissolved, they were rapidly injected into the first flask containing SnO solution. The temperature was then raised to 270 °C and kept for the range of 150 seconds to 500 seconds under vigorous stirring. The product was purified by standard polar/nonpolar solvent precipitation technique, using a high-speed centrifuge.

Ⅲ. Characterization. The crystal structure of SnSSe nanocrystals was characterized by powder X-ray diffraction (XRD) using Cu Kα radiation, λ=1.54 Å. An Oxford INCA energy-dispersive X-ray spectroscopy (EDS) detector was used to analyse element composition and proportion. Transmis-sion electron microscopy (TEM) and selected area electron diffraction(SAED) images were taken with a JEM 2100 microscope at 200 kV accelerating voltage. UV–vis absorption spectra were carried out to evaluate the optical properties of SnSSe nanocrystals by using a Lambda 20 UV–vis spectrometer.

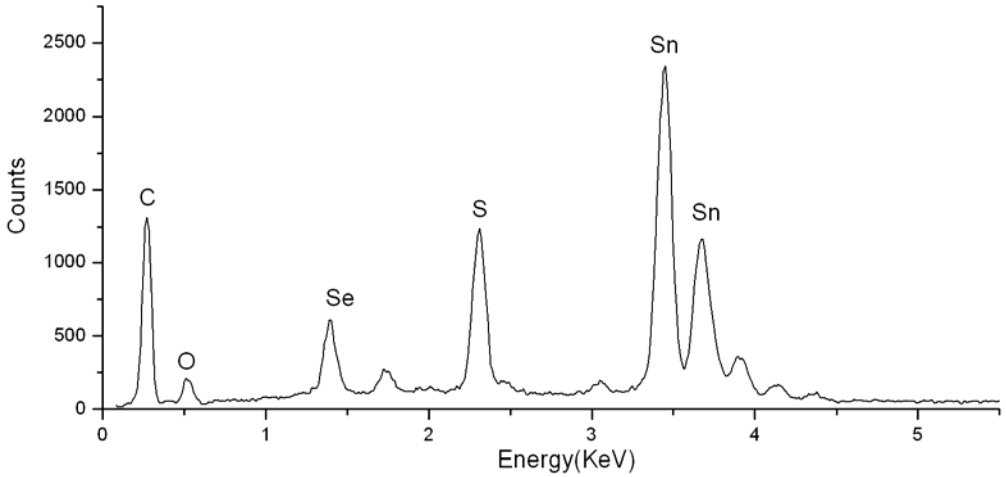

Fig. S1. EDS spectrum of SnS_xSe_{1-x} (x=0.75) nanocrystals.

Serials	S/(S+Se)	Atomic (%)		
		Sn	S	Se
I	0.09	53.8	4.3	41.9
II	0.22	52.4	10.5	37.1
III	0.43	52.4	20.4	27.2
IV	0.56	51.8	26.9	21.3
V	0.78	51.0	38.3	10.7
VI	0.89	51.0	43.9	5.1

Table S1. Chemical compositions of SnSSe nanocrystals determined from EDS analysis.

Table S1. shows the chemical stoichiometries of Six SnSSe samples measured by an Oxford INCA energy-dispersive X-ray spectroscopy (EDS) detector. The whole samples have an S/(S+Se) ratio of 0.09, 0.22, 0.43, 0.56, 0.78, 0.89. Considering the ±2% uncertainty in the elemental composition data analyzed by EDS, the average compositions of the nanocrystals for the six samples calculated from Table SI.1 are $SnS_{0.08}Se_{0.78}$, $SnS_{0.20}Se_{0.71}$, $SnS_{0.39}Se_{0.52}$, $SnS_{0.52}Se_{0.41}$, $SnS_{0.75}Se_{0.21}$ and $SnS_{0.86}Se_{0.10}$, respectively.

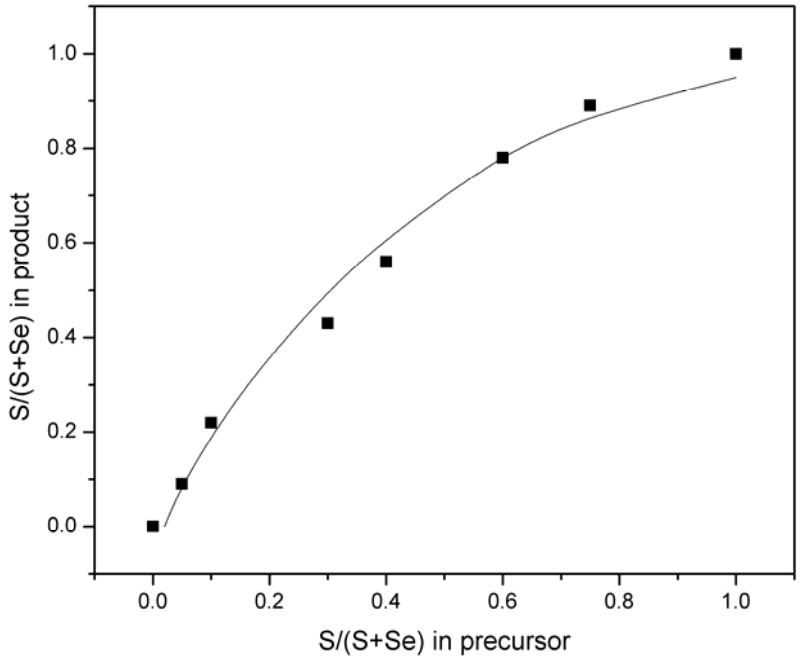

Fig. S2. Energy-dispersive X-ray spectroscopy (EDS) is used to measure the relative amount of sulfur in the product versus the relative amount of sulfur in the precursor injection solution.

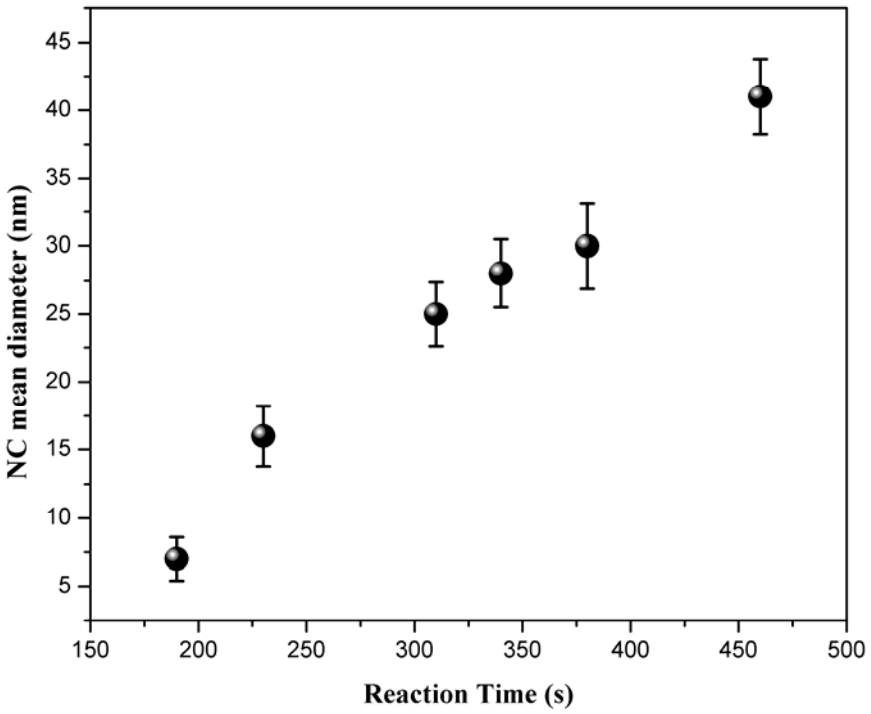

Fig. S3. Dependence of final particle size on the reaction time. The error bars describe the distribution of particle sizes within the sample, not the uncertainty in the mean.

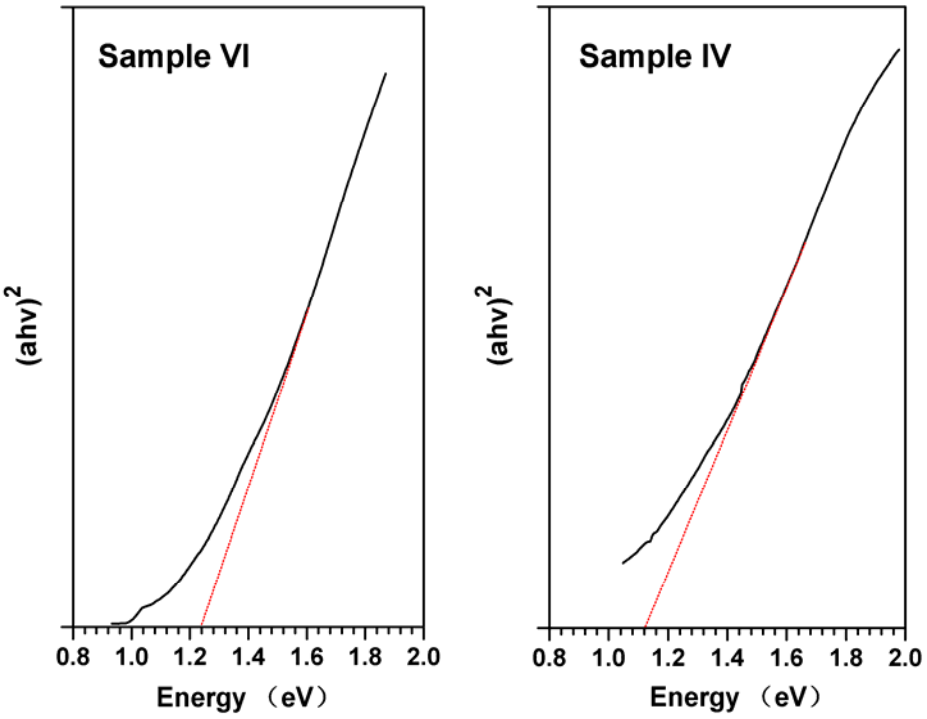

Fig. S4. Obtained band gap energies of Sample VI and Sample IV.