Electronic Supplementary Information (ESI)

Shape and stoichiometry control of bismuth selenide nanocrystals in colloidal synthesis

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Experimental Details

Chemical reagent:

$Bi(NO_3)_3 \cdot 5H_2O$ (≥99.0), oleyl amine (80%-90%) and Se powder (≥99.9) were obtained from Shanghai Jingchun Co/ Ltd.

Preparation for Bi_2Se_3, Bi_8Se_9 and $Bi_{1.007}Se_{0.993}$ films:

Bi_2Se_3, Bi_8Se_9 and $Bi_{1.007}Se_{0.993}$ nanocrystals were dissolved in toluene solution. To prepare films for photoelectrochemical tests, 0.2-0.3 mL solution of the materials was coated on ITO glass, respectively. Then the samples were kept in the draught cupboard to naturally evaporate toluene.

Materials characterizations

TEM images were obtained on a JEM-2100F field-emission transmission electron microscope with a working voltage of 200 kV. X-ray diffraction analysis was performed with rigaku-3014; X-Ray Fluorescence data were obtained from Shimadzu XRF-1800. The optical absorption spectra were collected using a Hitachi U-4100 spectrophotometer. X-ray photoelectron spectroscopy (XPS) analysis was performed with the Spectrometer of Thermo-VG Scientific ESCALAB 250Xi. The photoelectrochemical characterization was carried out in 0.1 M Na_2SO_4 solution in a Pyrex electrolytic cell. A 300 W xenon lamp was used as the light source, and the light intensity was kept at 40 mW/cm^2.

Table 1. XRF analysis of Bi_2Se_3, Bi_8Se_9 and $Bi_{1.007}Se_{0.993}$.

	Bi(At%)	Se(At%)	Bi:Se(At%)
Bi_2Se_3	40.71	59.28	4.1:6
Bi_8Se_9	45.66	54.33	5.1:6
$Bi_{1.007}Se_{0.993}$	50.26	49.73	1:1

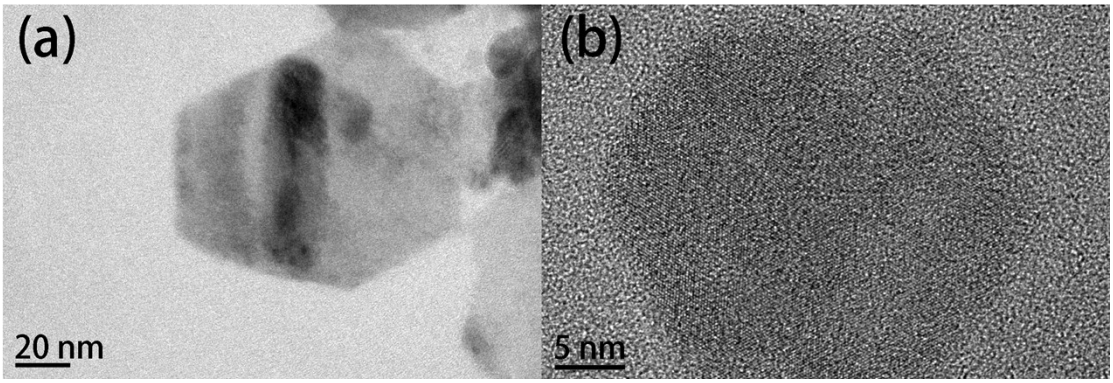

Fig. S1 (a)TEM and (b)HRTEM images of hexagonal Bi_2Se_3.

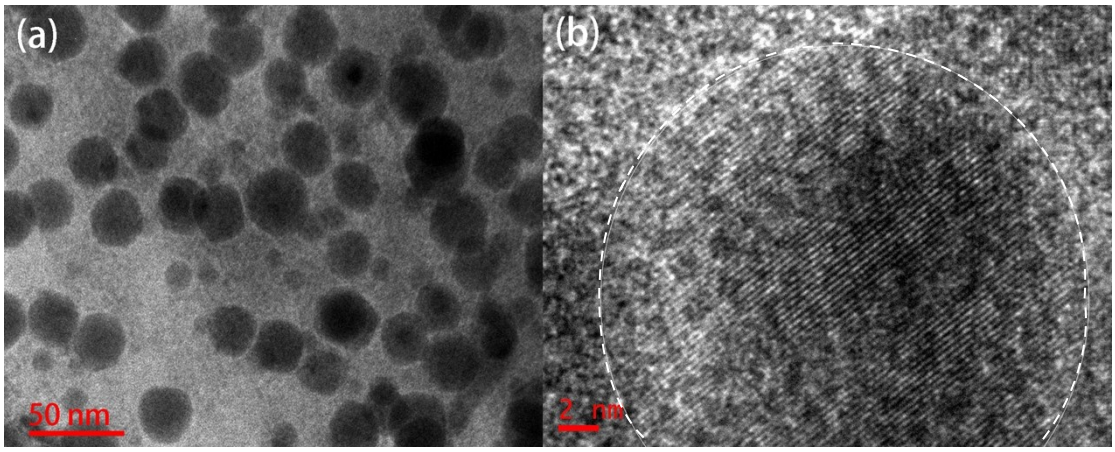

Fig. S2 (a)TEM and (b)HRTEM images of disk-like Bi_8Se_9.

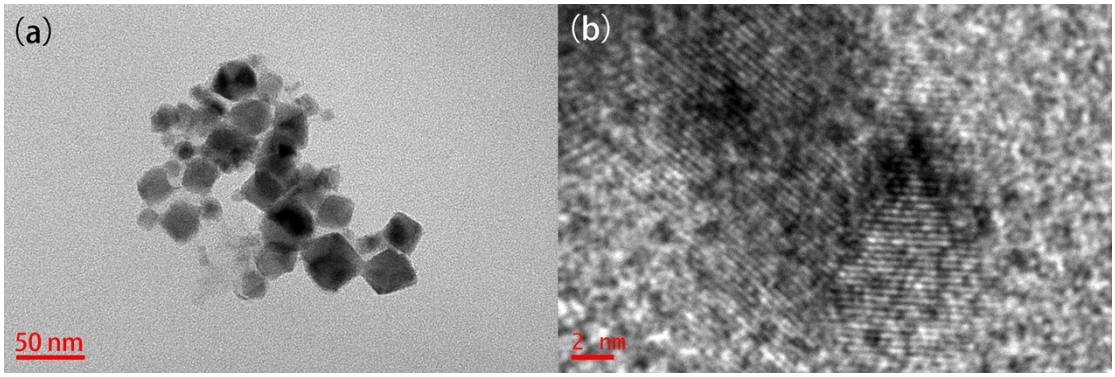

Fig. S3 (a)TEM and (b)HRTEM images of octahedron-like $Bi_{1.007}Se_{0.993}$.

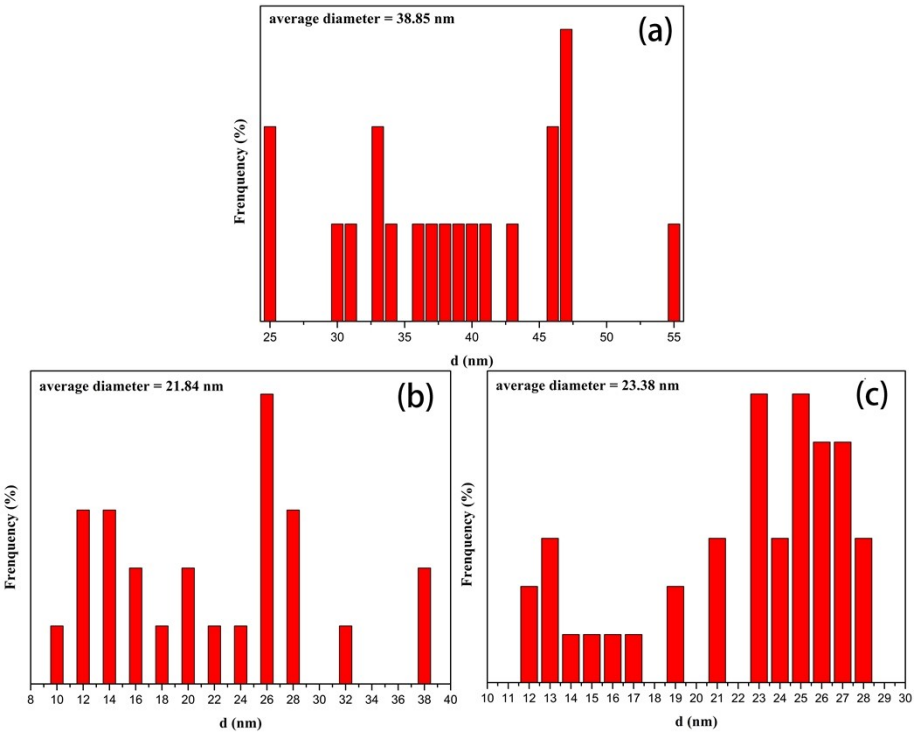

Fig. S4 Crystal size distribution of (a)Bi_2Se_3, (b)Bi_8Se_9 and (c)$Bi_{1.007}Se_{0.993}$.

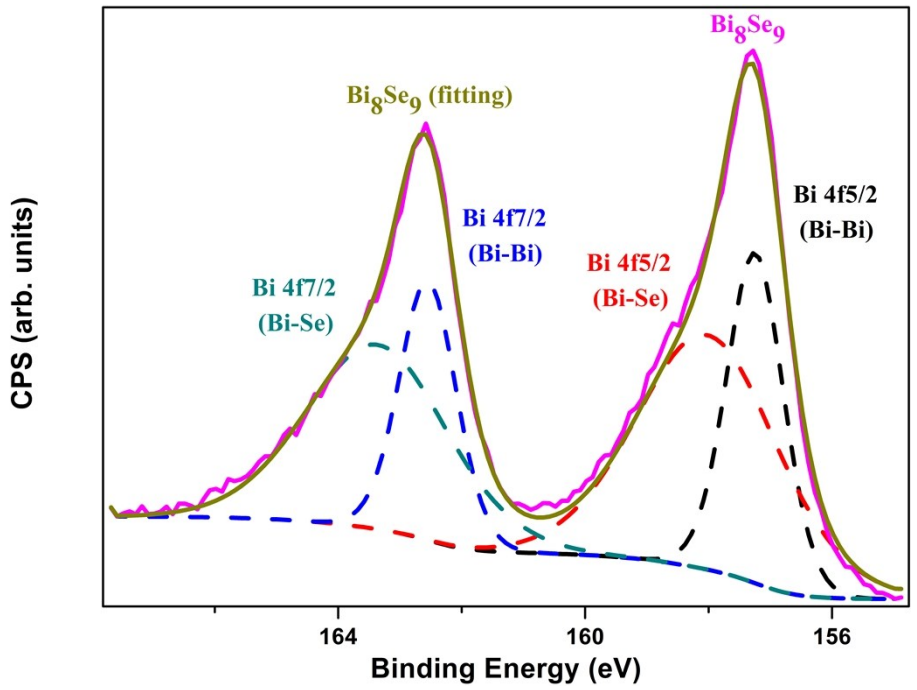

Fig. S5 XPS spectra of Bi 4f for Bi_8Se_9.

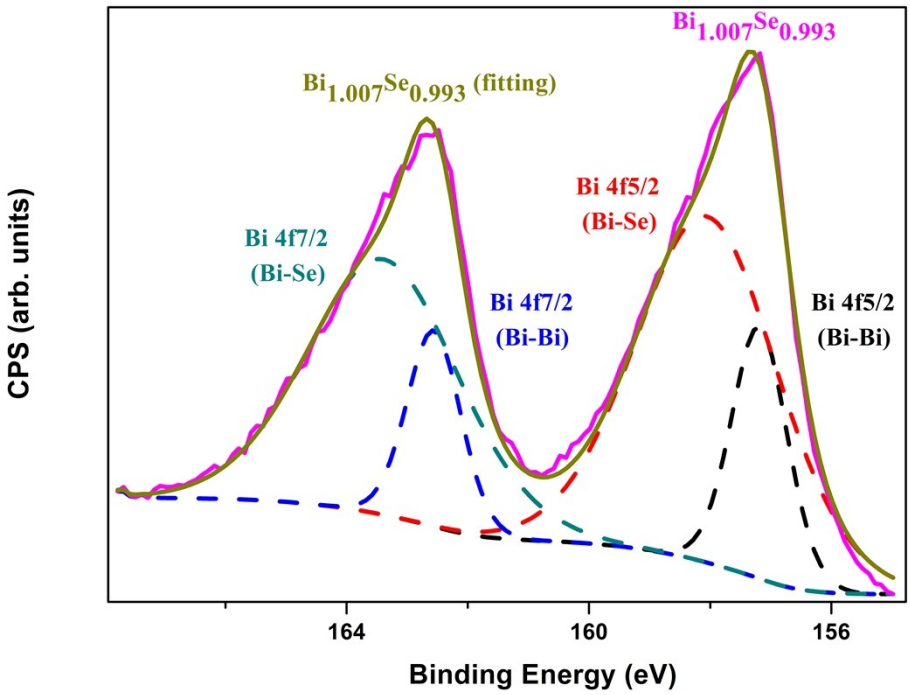

Fig. S6 XPS spectra of Bi 4f for $Bi_{1.007}Se_{0.993}$.

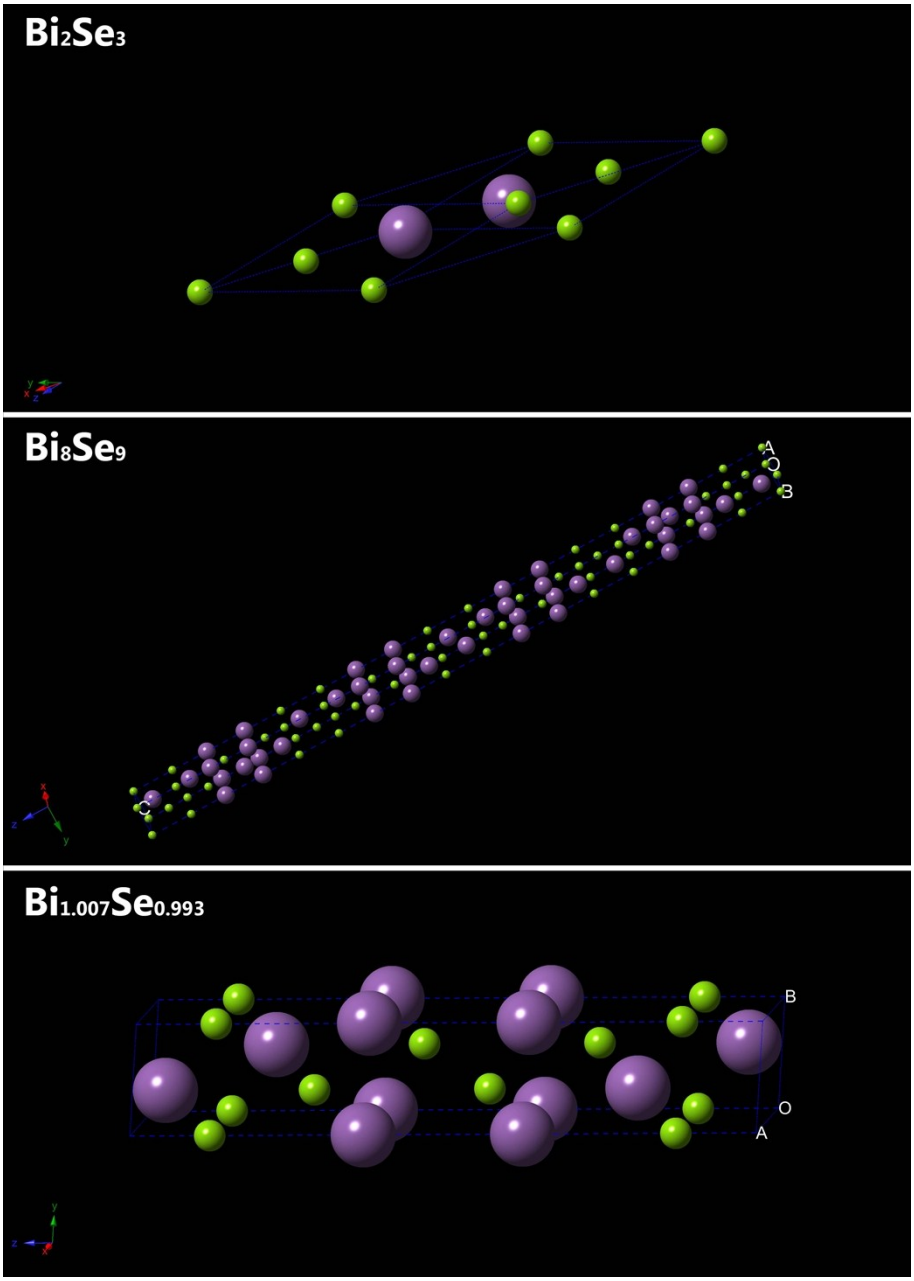

Fig. S7 Simulated single crystal structure of Bi_2Se_3, Bi_8Se_9 and $Bi_{1.007}Se_{0.993}$. Purple ball represents Bi atom and green ball represents Se atom.

Fig. S8 Bi-precursors kept at 220 °C, 250 °C and 290 °C.

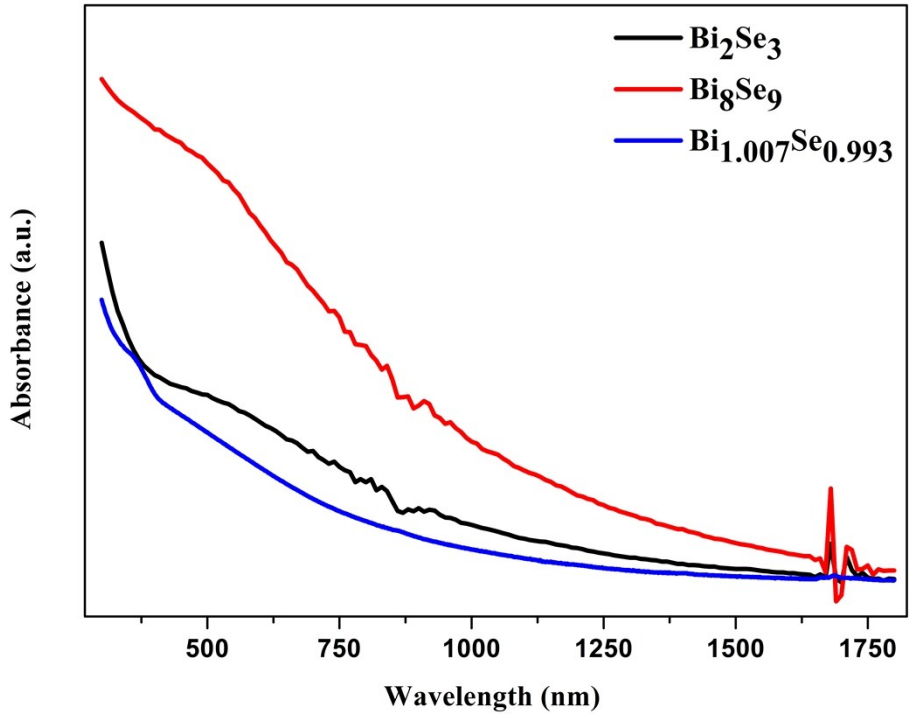

Fig. S9 Optical absorbance spectra of Bi_2Se_3, Bi_8Se_9 and $Bi_{1.007}Se_{0.993}$.

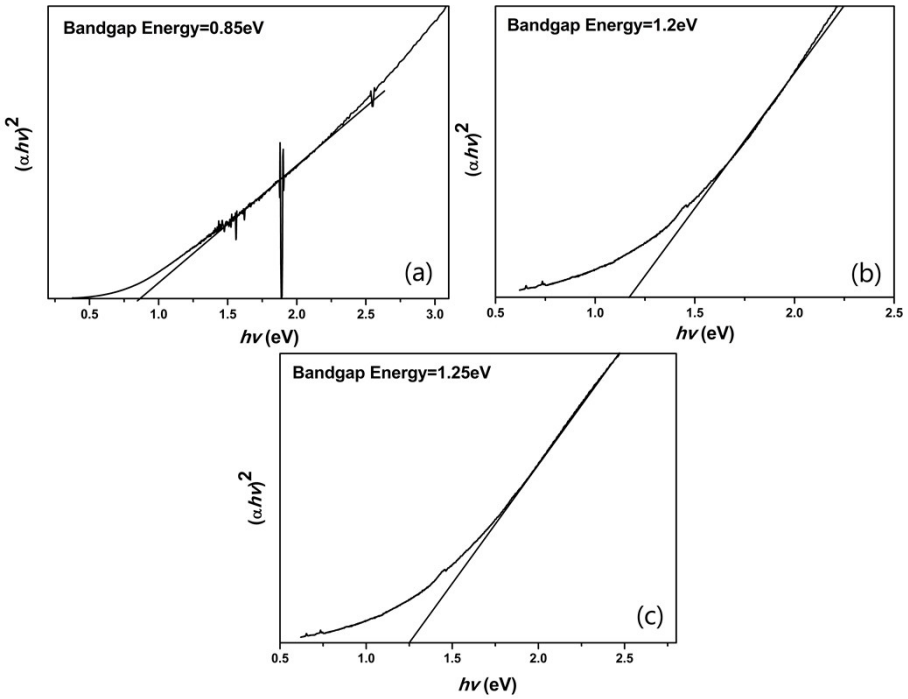

Fig. S10 Bandgap values of (a)Bi_2Se_3, (b)Bi_8Se_9 and (c)$Bi_{1.007}Se_{0.993}$.

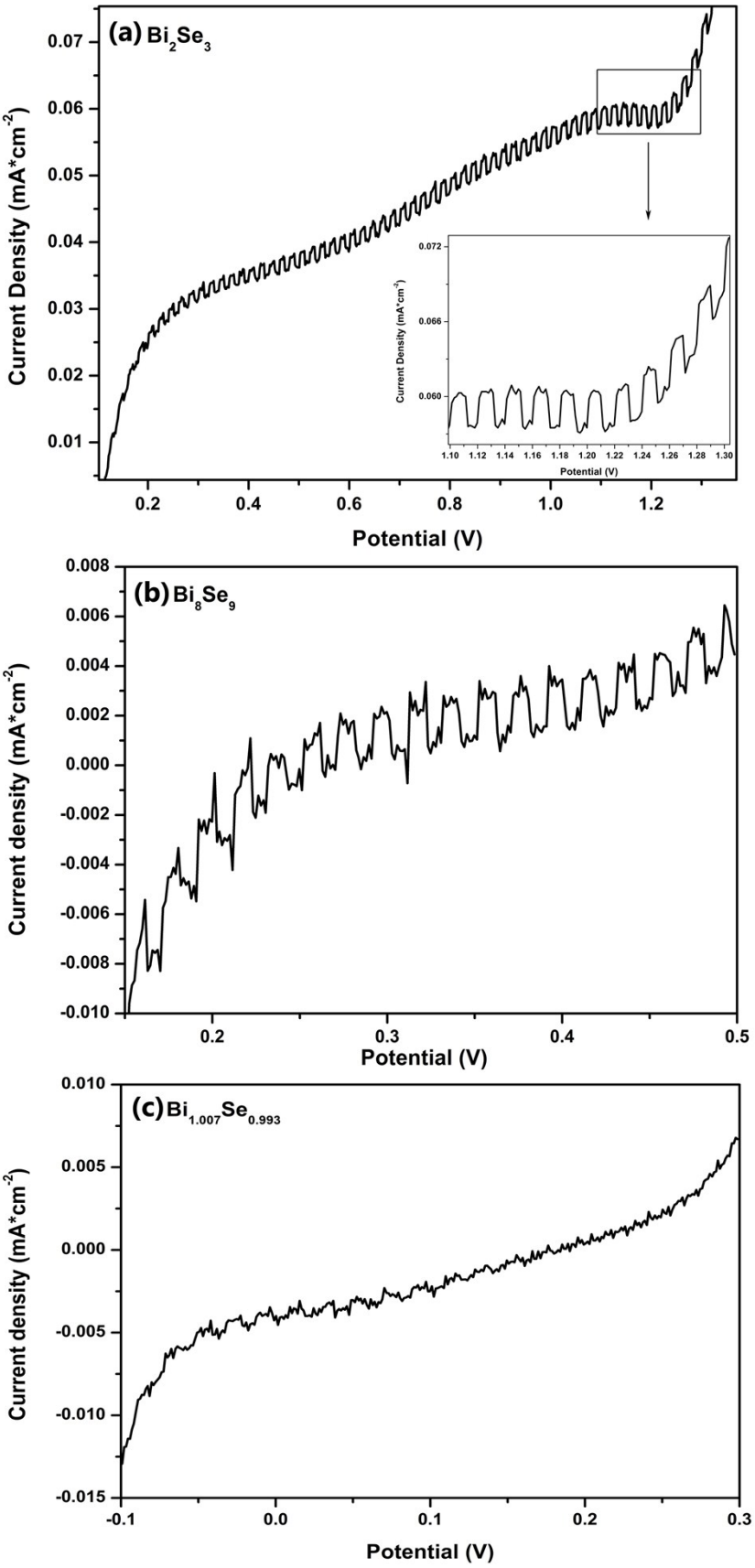

Fig. S11 J-V curves of (a) Bi_2Se_3, (b) Bi_8Se_9 and (c) $Bi_{1.007}Se_{0.993}$.