Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Enhanced thermoelectric performance of Cu_3SbS_4 flower-like hierarchical architectures composed of Cl doped nanoflakes via an in situ generated CuS template

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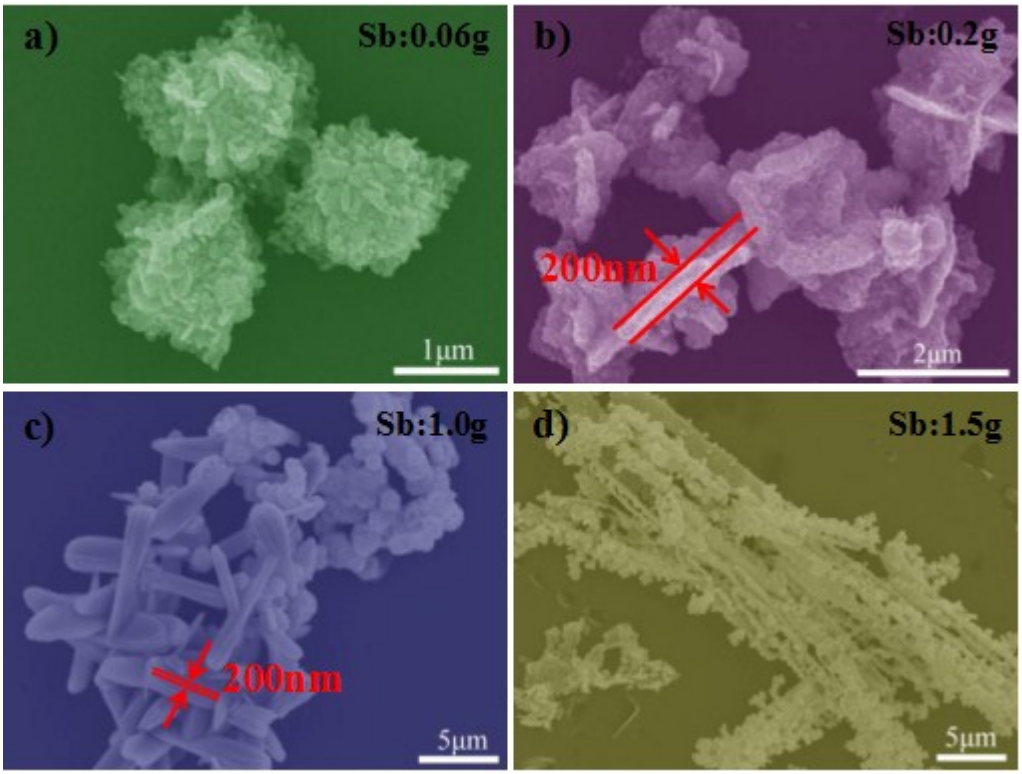

Fig.S1. SEM images of as-prepared samples synthesized with different amounts of Sb source (a-d) 0.06 g (0.09 mmol); 0.2 g (0.30 mmol); 1.0 g (1.48 mmol); 1.5 g (2.22 mmol), respectively.

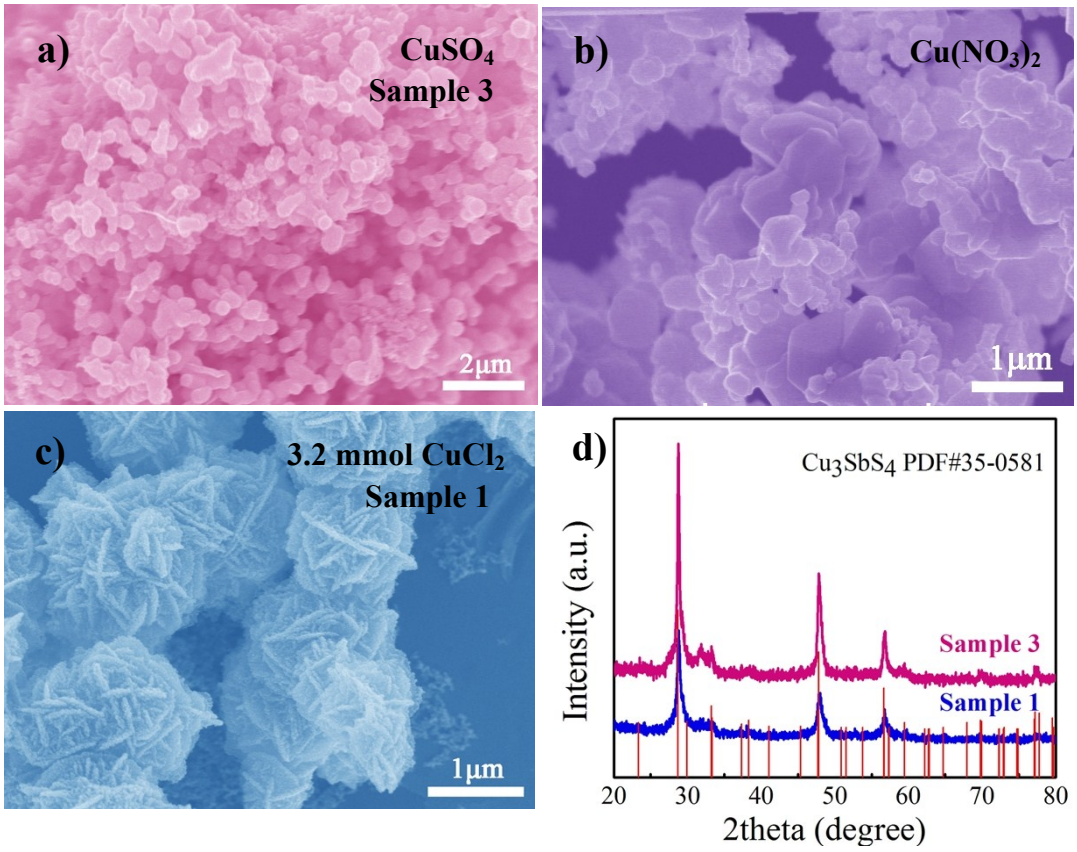

Fig.S2. SEM images of samples obtained by solvothermal treatment after introducing (a) $CuSO_4$ (Sample 3), (b) $Cu(NO_3)_2$ and (c) 3.2 mmol $CuCl_2$ as Cu precursor (Sample 1), respectively. (d) The corresponding XRD patterns of Sample 1 and 3.

Table S1. Lattice parameters (a and c), chemical composition, band gap of the Cl-free and Cl-doped Cu_3SbS_4 at 300 K. The values in parentheses are the statistical errors. Other errors such as temperature fluctuations (<1 K) should be considered for a and c.

Sample	Lattice parameters(Å) a	c	Cl adding amount	chemical composition	band gap (eV)
Sample 1	5.3842(1)	1.0764(2)	3.2mmol	$Cu_{3.8}SbS_{3.8}Cl_{0.9}$	1.06
Sample 2	5.3841(3)	1.0763(1)	1.6mmol	$Cu_{3.2}SbS_{3.8}Cl_{0.3}$	1.09
Sample 3	5.3840(2)	1.0762(2)	0 mmol	$Cu_{2.8}SbS_{3.8}$	0.98

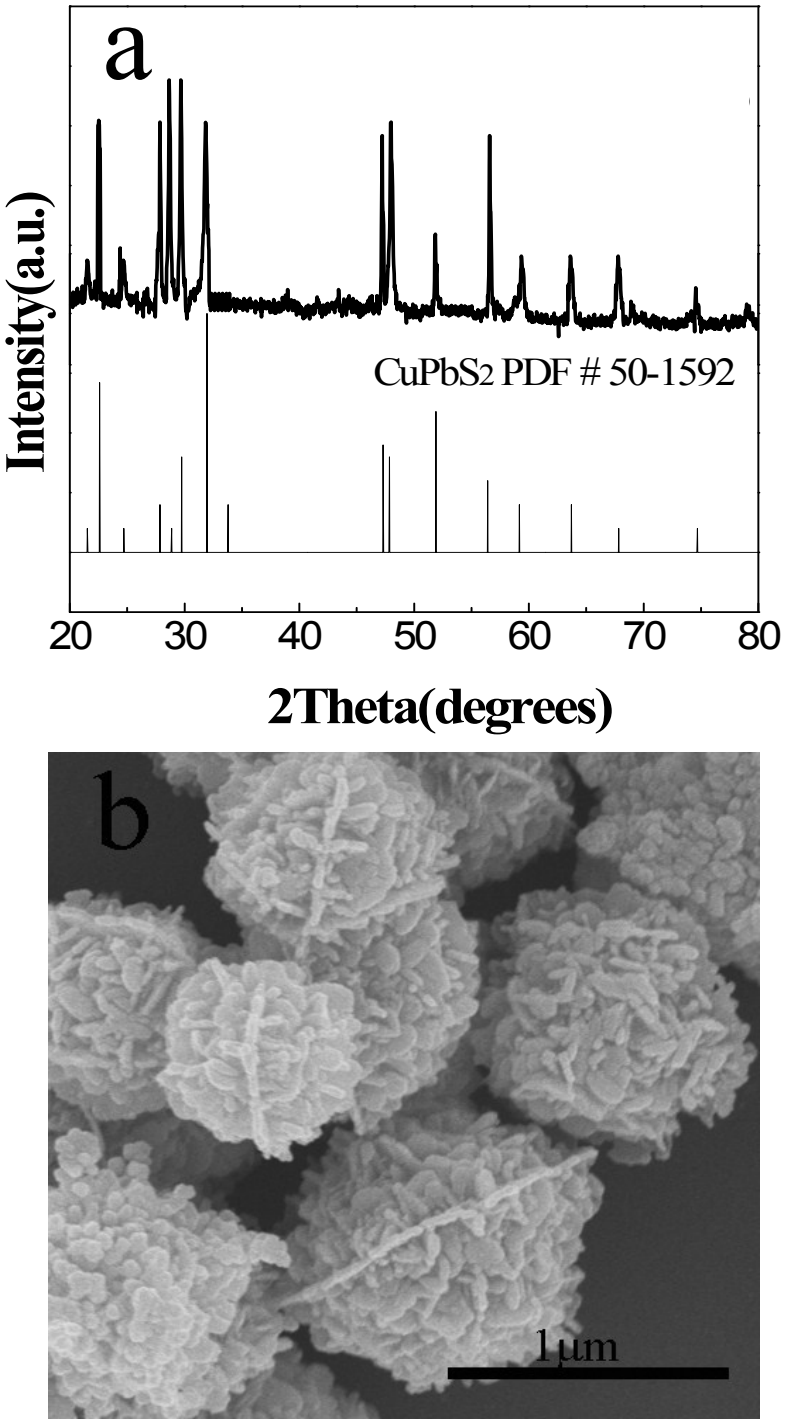

Fig. S3 Powder X-ray diffraction pattern (a) and SEM image (b) of $CuPbS_2$ microspheres.

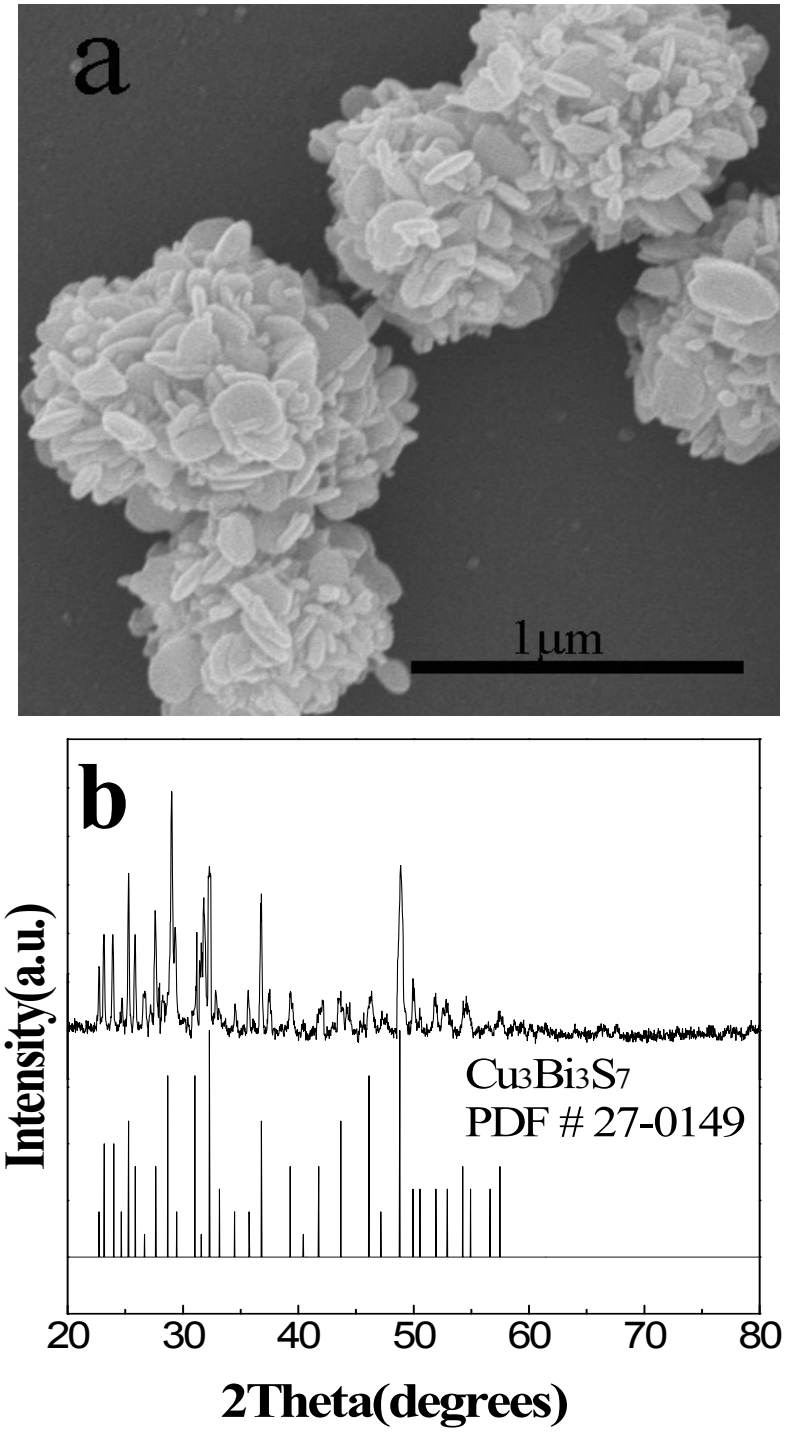

Fig. S4 SEM image (a) and powder X-ray diffraction pattern (b) of $Cu_3Bi_3S_7$ microspheres.

Table S2. A summary of *n* or *p* type semiconductor conduction behavior, room temperature Hall carrier concentration (n_H), and mobility (μ_H) of the Cl-doped Cu_3SbS_4 pellets.

Pellet	Cl adding amount	behavior	n_H [cm^{-3}]	μ_H [$cm^2V^{-1}s^{-1}$]
Sample 2	1.6mmol	p-type	3.9×10^{19}	1.87
Sample 4	6.4mmol	n-type	2.2×10^{20}	0.32