Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2015

## Electronic Supplementary Information

Thermoelectric performance of SnS and $\mathrm{SnS}-\mathrm{SnSe}$ solid solution

Ye-Mao Han, $\psi^{a, b}$ Jie Zhao, $\ddagger^{a, b}$ Min Zhou, ${ }^{* a}$ Xing-Xing Jiang, ${ }^{b, c}$, Hua-Qian Leng, ${ }^{a, b}$ Lai-Feng Li ${ }^{*}{ }^{*}$<br>$a$ Key Laboratory of Cryogenics, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China<br>$b$ University of Chinese Academy of Sciences, Beijing 10049, China<br>$c$ Beijing Center for Crystal R\&D, Key Lab of Functional Crystals and Laser Technical of Chinese Academy of Sciences, Technical Institute of Physics and<br>Chemistry, CAS, Beijing, 100190, China.

$\dagger$ These authors contributed equally to this work.

* Corresponding Authors
mzhou@mail.ipc.ac.cn
laifengli@mail.ipc.ac.cn

1. The heat capacity of $\mathrm{SnS}_{1-\mathrm{x}} \mathrm{Se}_{\mathrm{x}}$ solid solution.


Figure S 1 . The heat capacity $\left(\mathrm{C}_{\mathrm{P}}\right) \operatorname{SnS}_{1-\mathrm{x}} \mathrm{Se}_{\mathrm{x}}(\mathrm{x}=0,0.2,0.5,0.8,1.0)$ solid solution. $\mathrm{The}_{\mathrm{p}}$ of SnS and SnSe are obtained from Orr an Zhao's works. ${ }^{1,2}$ The $\mathrm{C}_{\mathrm{P}}$ of $\mathrm{SnS}_{1-\mathrm{x}} \mathrm{Se}_{\mathrm{x}}(\mathrm{x}=0.2,0.5,0.8)$ was calculated by linear fitting from $\mathrm{C}_{\mathrm{p}}$ of SnS and SnSe .

## 2. The orientation factor calculation

The orientation factor calculation can be expressed as:
$F=\frac{1-P}{1-P_{0}}$,
where P and $\mathrm{P}_{0}$ can be calculated from the experiment data and the refinement documents. ${ }^{3}$
The P and $\mathrm{P}_{0}$ can be expressed as below:
$P=\frac{\sum I(h 00)}{\sum I(h k l)}$,
and $P_{0}=\frac{\sum I_{0}(h 00)}{\sum I_{0}(h k l)}$.
Here $\mathrm{I}(\mathrm{h} 00)$ is the peak intensity of (h00) planes and $\mathrm{I}(\mathrm{hkl})$ is the peak intensity of all peaks. $\mathrm{I}_{0}(\mathrm{~h} 00)$ is the peak intensity of $(\mathrm{h} 00)$ and $\mathrm{I}_{0}(\mathrm{hkl})$ is the peak intensity of (hkl) according to cell refinement data. In cell refinement data, all the peaks was seen to emerge for equal possibility.

Table S 1 . The orientation factors of $\mathrm{SnS}_{1-\mathrm{x}} \mathrm{Se}_{\mathrm{x}}$ solid solution. The data of SnSe got from ref. 4.

| Sample | Orientation Factor |  |  |
| :---: | :---: | :---: | :---: |
|  | Powder | $\\|$ pressuring direction | $\perp$ pressuring direction |
| $\mathrm{SnS}^{\prime}$ | 0.66 | 0 | 0.22 |
| $\mathrm{SnS}_{0.2} \mathrm{Se}_{0.8}$ | 0.72 | 0 | 0.26 |
| $\mathrm{SnS}_{0.5} \mathrm{Se}_{0.5}$ | 0.72 | 0 | 0.30 |
| $\mathrm{SnS}_{0.8} \mathrm{Se}_{0.2}$ | 0.68 | 0 | 0.20 |
| $\mathrm{SnSe}^{4}$ | 0.69 | 0 | 0.32 |

3. Thermoelectric performances $\mathrm{SnS}_{0.2} \mathrm{Se}_{0.8}$

The thermoelectric properties of $\mathrm{SnS}_{0.2} \mathrm{Se}_{0.8}$ along two directions were shown in Fig. 3. Compared to $\perp$ direction, the electrical resistivity ( $\rho$ ) and Seebeck coefficient (S) are higher and the thermal conductivity ( $\kappa$ ) is lower along $\|$ direction. The difference in $\rho, S$ and $\kappa$ comes from the preferred orientation of (400) plane and it has the lowest carrier mobility $(\mu)$ and lattice thermal conductivity $\left(\kappa_{\mathrm{L}}\right) .{ }^{2}$ Unlike the great difference of electrical resistivity and thermal conductivity along two directions, the difference of Seebeck coefficient along two directions was small and the Seebeck coefficient along parallel to pressing direction is little higher than the Seebeck coefficient along perpendicular to pressing direction. Although the electrical properties along $\|$ direction are lower than $\perp$ direction, the lower $\kappa$ along $\|$ direction than $\perp$ direction is beneficial to the thermoelectric performance along \| direction, and higher zT of 0.82 was reached along $\|$ direction than zT of 0.62 along $\perp$ direction. Therefore, the thermoelectric performance along $\|$ direction is higher than along $\perp$ direction.


Figure S 2 . Thermoelectric performance of $\mathrm{SnS}_{0.2} \mathrm{Se}_{0.8}$ at different temperature along different directions. (a) the Seebeck coefficient, (b) the electrical resistivity, (c) the thermal conductivity and lattice thermal conductivity and (d) the zT values.

## Reference:

1. R. Orr and A. Christensen, J. Phys. Chem., 1958, 62, 124.
2. L. Zhao, S. Lo, Y. Zhang, H. Sun, G. Tan, C. Uher, C. Wolverton, V. Dravid and M. Kanatzidis, Nature, 2014, 508, 373.
3. F. Lotgering, J. Inorg. Nucl. Chem., 1959, 9, 113.
4. J. Zhao, M. Zhou, Y. Han, H. Leng, L. Li, Solid State Commun., 2014, Submitted.
