

Electronic Supporting Information

The p-n transformation and thermoelectric property optimization for $\text{Cu}_{1+x}\text{FeSe}_2$ ($x=0-0.05$) alloys

Jinze Zhai, Hongchao Wang, Wenbin Su, Teng Wang, Fahad Mehmood,
Xue Wang, Tingting Chen, Taichang Huo, Kaiqi Zhang, Chunlei Wang

School of Physics, State Key Laboratory of Crystal Materials, Shandong
University, Jinan 250100, P. R. China

*E-mail: wanghc@sdu.edu.cn (H. Wang),

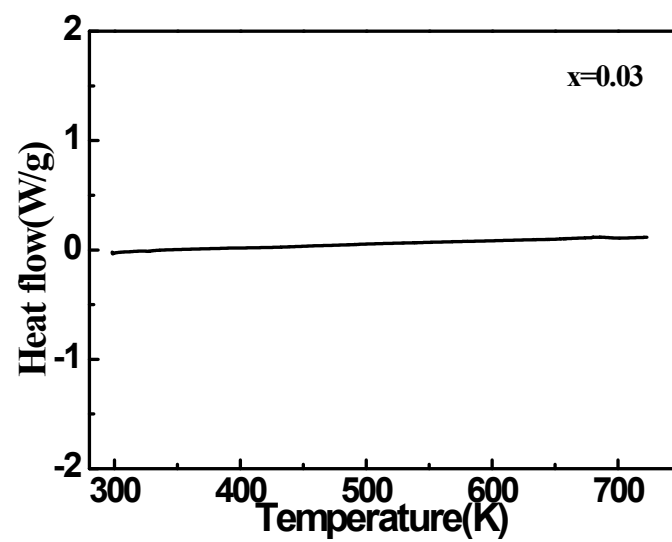
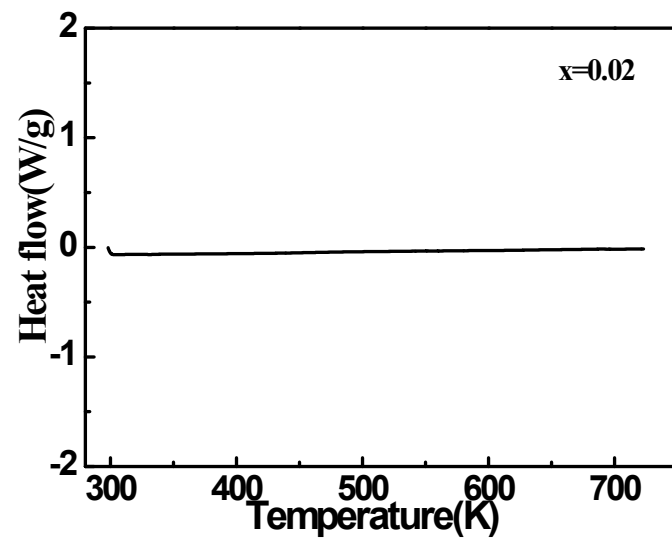
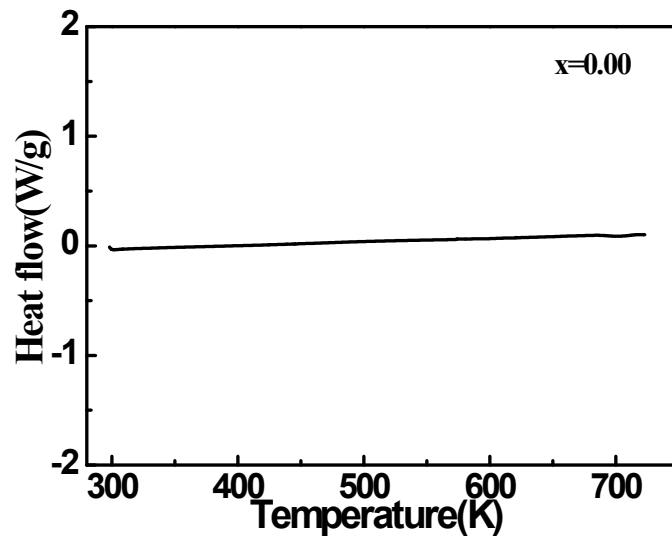
E-mail: wangcl@sdu.edu.cn (C. Wang)

Table S1. The theoretical, experimental and relative densities for all $\text{Cu}_{1+x}\text{FeSe}_2$ samples.

x	0.00	0.01	0.02	0.03	0.05
Theoretical density	5.544	5.545	5.562	5.548	5.553
Experimental density	5.413	5.195	5.159	5.212	5.060
Relative density	98%	94%	93%	93%	91%

Table S2. The Goldsmid-Sharp band gaps for all $\text{Cu}_{1+x}\text{FeSe}_2$ samples.

x	0.00	0.01	0.02	0.03	0.05
$E_{GS}(\text{eV})$	0.17	0.17	0.18	0.19	0.16



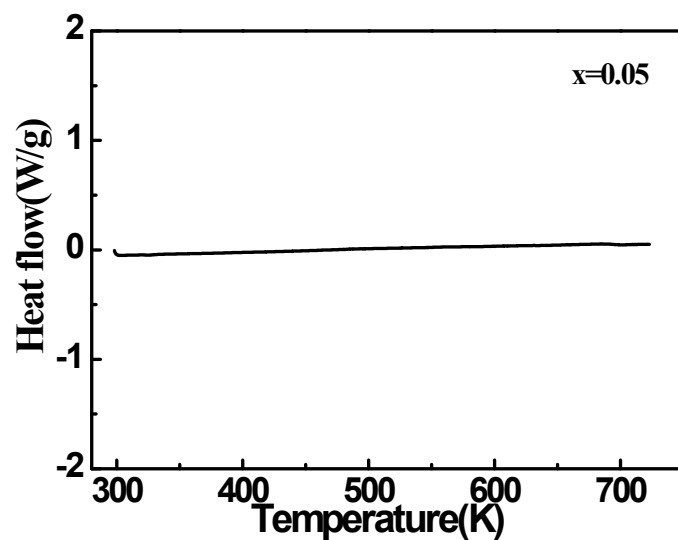


Figure S1. DSC data of $\text{Cu}_{1-x}\text{FeSe}_2$ ($x=0.00, 0.02, 0.03$ and 0.05) in temperature range of 300K-723K under N_2 atmosphere.