

Supplemental Information

Thermoelectric properties of $\text{Cu}_4\text{Ge}_3\text{Se}_5$ with an intrinsic disordered zinc blende structure

Bing Shan, Siqi Lin*, Zhonglin Bu, Jing Tang, Zhiwei Chen, Xinyue Zhang, Wen Li and Yanzhong Pei*

Interdisciplinary Materials Research Center, School of Materials Science and Engineering, Tongji Univ., 4800 Caoan Rd.,
Shanghai 201804, China.

*Email: linsiqi0811@163.com; yanzhong@tongji.edu.cn

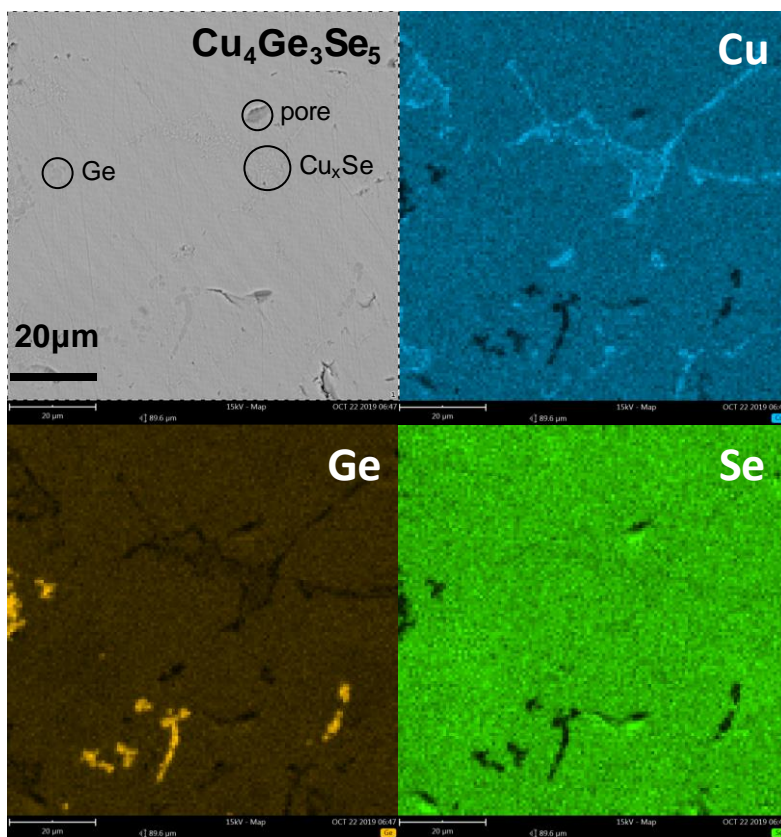


Figure S1. The SEM images for $\text{Cu}_4\text{Ge}_3\text{Se}_5$ with Ge and Cu_xSe precipitates.

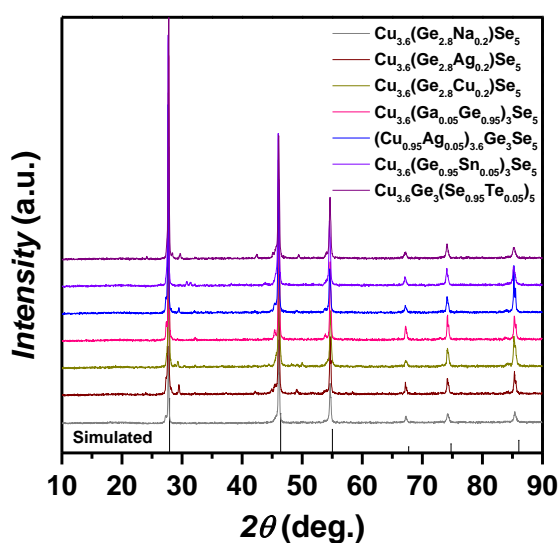


Figure S2. The XRD patterns for doped $\text{Cu}_{3.6}\text{Ge}_3\text{Se}_5$.

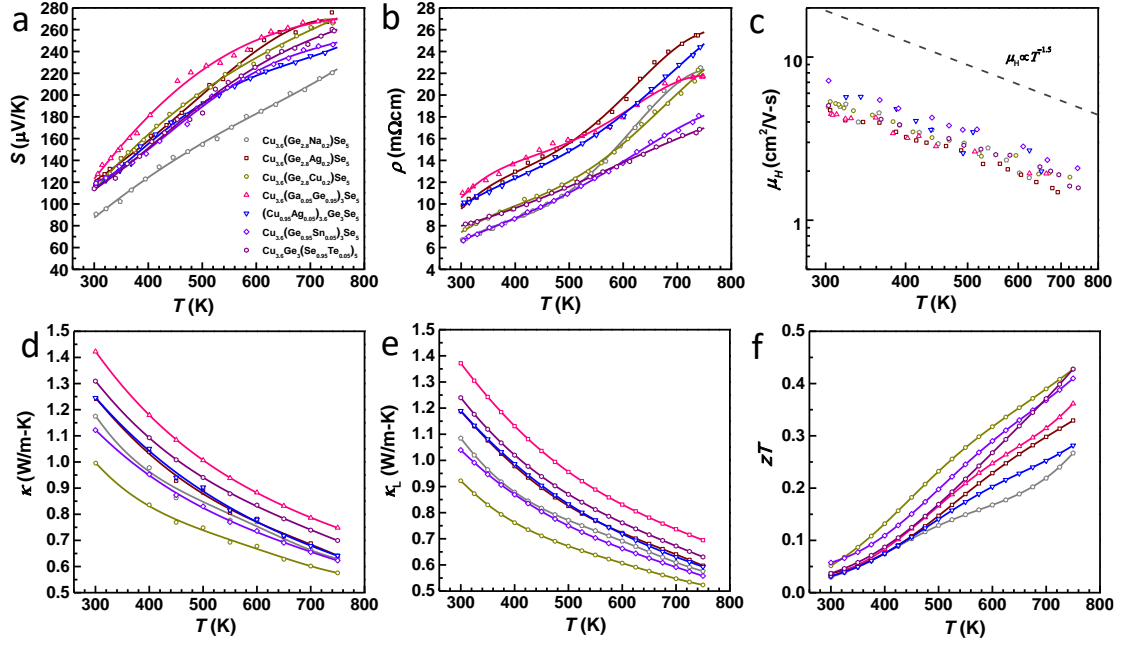


Figure S3. Temperature dependent Seebeck coefficient (a), resistivity (b), Hall mobility (c), total thermal conductivity (d) and lattice component (e), and zT (f) for doped $\text{Cu}_{3.6}\text{Ge}_3\text{Se}_5$.

Table S1. Room temperature Hall carrier concentration (n_H), transverse (v_t), longitudinal (v_l) and mean (v) sound velocities, bulk (B) and shear (G) modulus, Grüneisen parameter (γ) as well as Debye temperature (Θ_D) for doped $\text{Cu}_{3.6}\text{Ge}_3\text{Se}_5$.

Composition	n_H (10^{20} cm^{-3})	v_t (m/s)	v_l (m/s)	v (m/s)	B (GPa)	G (GPa)	γ	Θ_D (K)
$\text{Cu}_{3.6}(\text{Ge}_{2.8}\text{Ag}_{0.2})\text{Se}_5$	1.14	2130	4065	2382	57.6	25.0	1.8	253
$\text{Cu}_{3.6}(\text{Ge}_{2.8}\text{Cu}_{0.2})\text{Se}_5$	1.24	2146	3996	2396	53.0	24.8	1.8	253
$\text{Cu}_{3.6}(\text{Ga}_{0.05}\text{Ge}_{0.95})_3\text{Se}_5$	1.13	2273	4257	2539	62.0	28.5	1.8	270
$(\text{Cu}_{0.95}\text{Ag}_{0.05})_{3.6}\text{Ge}_3\text{Se}_5$	1.02	2128	4089	2381	58.6	24.9	1.9	252
$\text{Cu}_{3.6}(\text{Ge}_{0.95}\text{Sn}_{0.05})_3\text{Se}_5$	1.37	2252	4475	2525	73.2	28.0	2.0	268
$\text{Cu}_{3.6}\text{Ge}_3(\text{Se}_{0.95}\text{Te}_{0.05})_5$	1.56	2200	4215	2461	62.7	26.8	1.9	261