Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supplemental material:

Enhancement of thermoelectric performance of β-Zn_4Sb_3 through resonant distortion of electronic density of states doped with Gd

Baojin Ren,[a] Mian Liu,[a] Xiaoguang Li,[b] Xiaoying Qin,*[a] Di Li,[a] Tianhua Zou,[a] Guolong Sun,[a] Yuanyue Li,[a] Hongxing Xin,[a] and Jian Zhang[a]

[a]*Key Laboratory of Materials Physics, Institute of Solid State Physics,Chinese Academy of Science, 230031 Hefei, P. R. China.*

[b]*Hefei National Laboratory for Physical Sciences at Microscale, Department of Physics, University of Science and Technology of China, 230026 Hefei, P. R. China.*

Corresponding author. Tel: +86 0551 65592750; fax:+86 0551 65591434.
E-mail address: xyqin@issp.ac.cn.

(1) Microstructural characterization

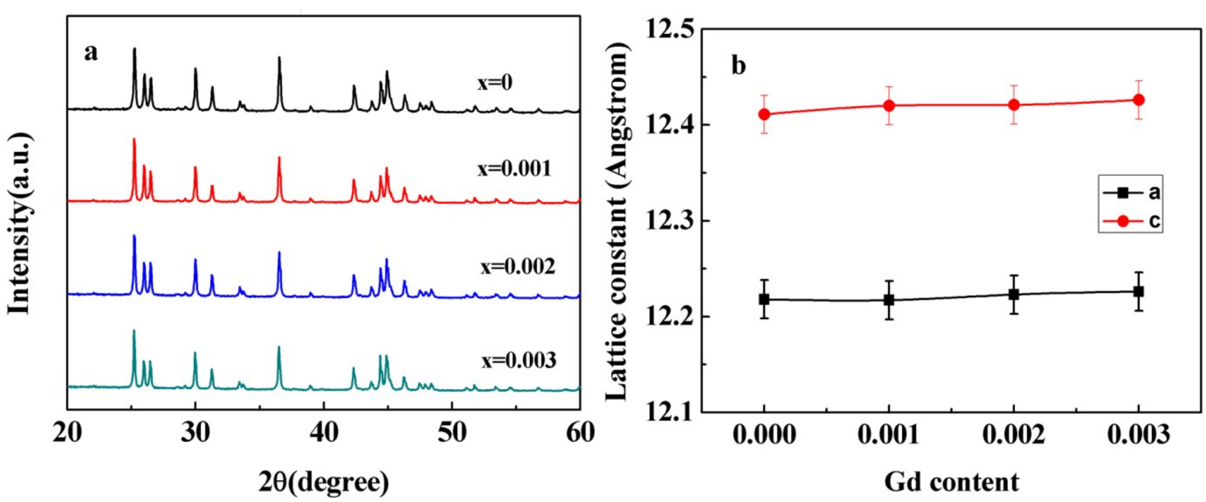

Fig. S1 (a) XRD patterns and (b) lattice constant of the β-$(Zn_{1-x}Gd_x)_4Sb_3$ (x=0, 0.001, 0.002 and 0.003) samples.

(2) Lattice thermal conductivity

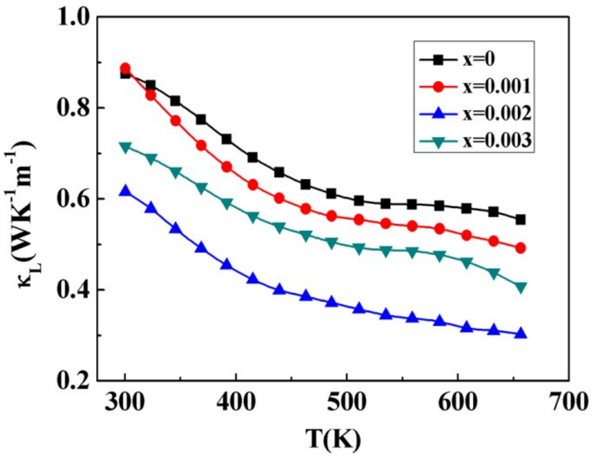

Fig. S2 Temperature dependences of lattice thermal conductivity κ_L.

(3) The heat capacity of part samples

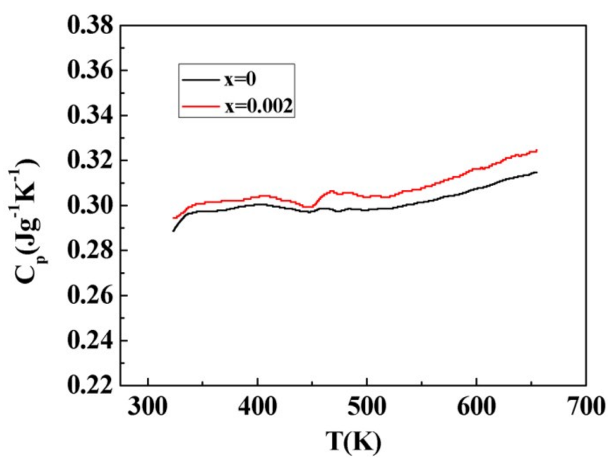

Fig. S3 Temperature dependences of heat capacity C_p for x = 0 and 0.002 compounds.

(4) The magnetic contributions C_m from Gd

The magnetic contributions C_m from 4f electrons of Gd cannot be ignored in Gd-doped samples**.** M.J. Parsons *et al.*[1, 2] have calculated the magnetic entropy S_m of Gd, which has proportional relationship with both temperature and Gd content at T<9 K. According to relationship between entropy S_m and heat capacity C_m: $C_m = T\frac{dS_m}{dT}$, the magnetic heat capacity contribution C_m for the sample with x=0.002 can be derived as: $C_m=3.6T$ *(mJ/mol. K)*. Then total heat capacity for the Gd-doped samples should be written as $C_p=\gamma T+bT^3+C_m$, *or* $C_p-C_m=\gamma T+bT^3$. (see Fig. S4)

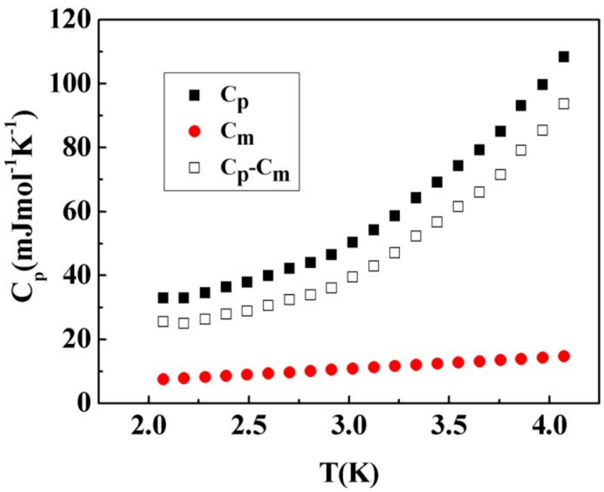

Fig. S4 Temperature dependence of C_p, C_m and C_p-C_m for x=0.002 sample.

Reference

1. M. J. Parsons, J. Crangle, B. Dennis, K. U. Neumann and K. R. A. Ziebeck, *Czech J Phys*, 1996, **46**, 2057-2058.
2. M. J. Parsons, J. Crangle, K. U. Neumann and K. R. A. Ziebeck, *J Magn Magn Mater*, 1998, **184**, 184-192.