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

Enhancing the thermoelectric performance of Cu_2Se by doping Te

Yong-Bin Zhu [a], Bo-Ping Zhang [a†], and Yong Liu [b]

[a] *The Beijing Municipal Key Laboratory of New Energy Materials and Technologies, School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, 100083, China.*

[b] *AECC Beijing Institute of Aeronautical Materials, Beijing, 100095, China.*

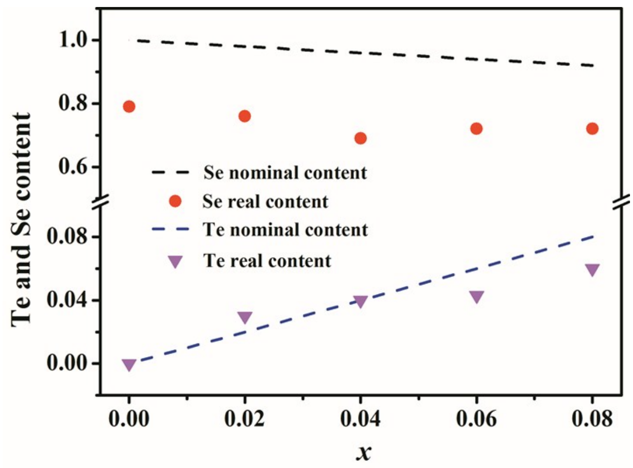

Fig. S1. The Te, Se nominal and real content dependence of the Te doping content x in the $Cu_2Se_{1-x}Te_x$ bulk samples.

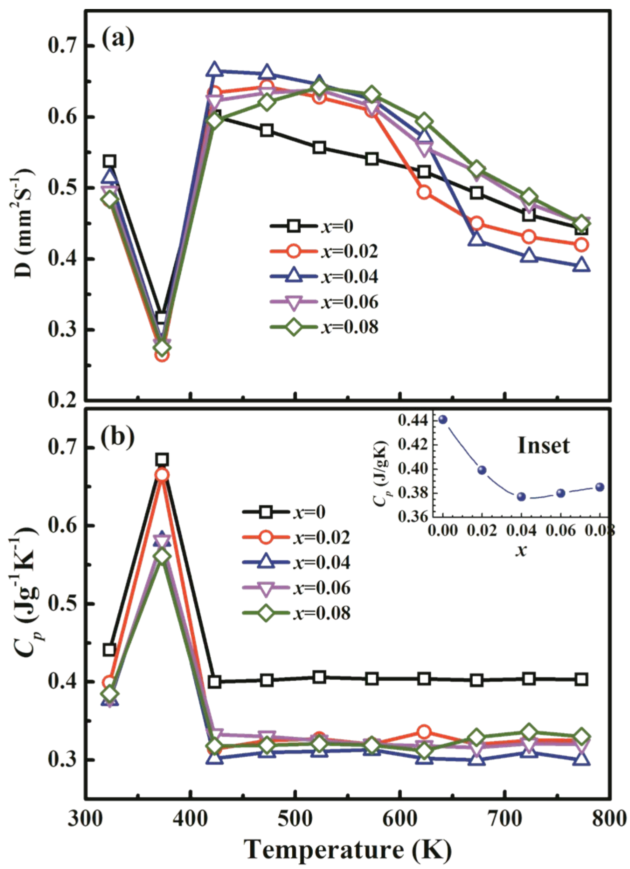

Fig. S2. Temperature dependence of the thermal transport property of $Cu_2Se_{1-x}Te_x$. (a) thermal diffusion coefficient (D), (b) special heat (C_p), the inset show the C_p dependent on Te-doped content (x) at 323 K.

The Lorenz number (Eq. (1)) varies was calculated via using Reduced Fermi energy (η), which is one-to-one correspondence with Seebeck coefficient (S) value. According to the traditional single parabolic band model, η implicitly determined by the S (Eq. (2)) was used to estimate the L.

$$L = \left(\frac{\kappa_B}{e}\right)^2 \left\{ \frac{\left(r+\frac{7}{2}\right)F_{\left(r+\frac{5}{2}\right)}(\eta)}{\left(r+\frac{3}{2}\right)F_{\left(r+\frac{1}{2}\right)}(\eta)} - \left[\frac{\left(r+\frac{5}{2}\right)F_{\left(r+\frac{3}{2}\right)}(\eta)}{\left(r+\frac{3}{2}\right)F_{\left(r+\frac{1}{2}\right)}(\eta)}\right]^2 \right\} \quad (1)$$

$$S = \frac{\kappa_B}{e}\left[\frac{\left(r+\frac{5}{2}\right)F_{\left(r+\frac{3}{2}\right)}(\eta)}{\left(r+\frac{3}{2}\right)F_{\left(r+\frac{1}{2}\right)}(\eta)} - \eta\right] \quad (2)$$

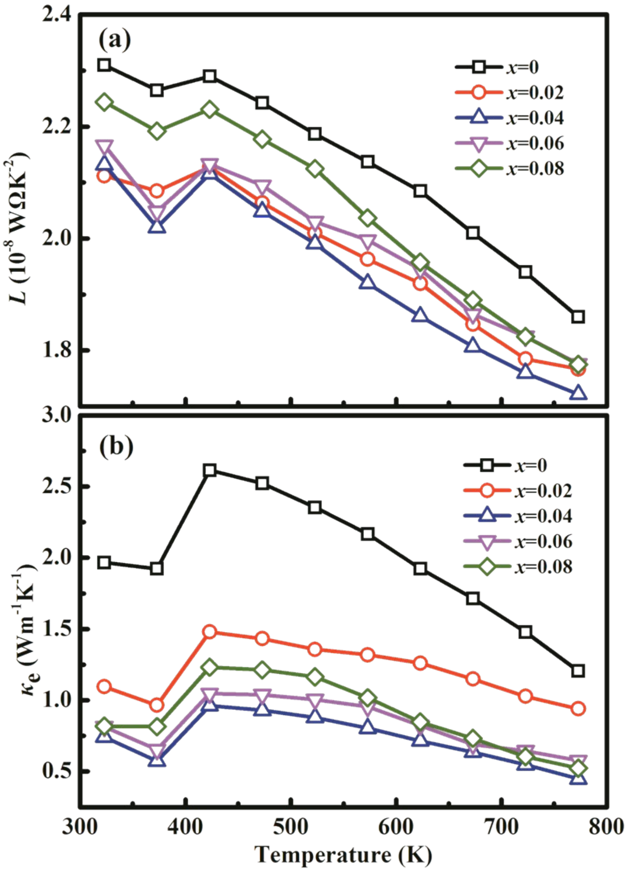

Fig. S3. The calculated Lorenz number (L) (a), and carrier thermal conductivity (κ_e) (b), for $Cu_2Se_{1-x}Te_x$ samples dependent on the temperature, based on the SPB model.