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Ag doping induced abnormal lattice thermal conductivity in Cu_2Se

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1. Rietveld refinement calculated Cu_2O content and its influence on thermoelectric performance of Cu_2Se

Figure S1a and b show the experimental XRD patterns in comparison with the Rietveld refinement calculated ones of as-sintered $(Cu_{1-x}Ag_x)_2Se$ pellets and the calculated the Cu_2O ratios. The R_{wp} values for $(Cu_{1-x}Ag_x)_2Se$ with x=0, 0.005 and 0.01 are 7.9, 6.8 and 7.2 %, respectively. As can be seen, with increasing the Ag-doping level, the Cu_2O content increases up to 3.5 *at.* %. This fraction is lower than the critical point of ~7 *at.* %.[1] Below this point, Cu_2O has minor influence on thermoelectric performance of as-prepared $(Cu_{1-x}Ag_x)_2Se$.[1]

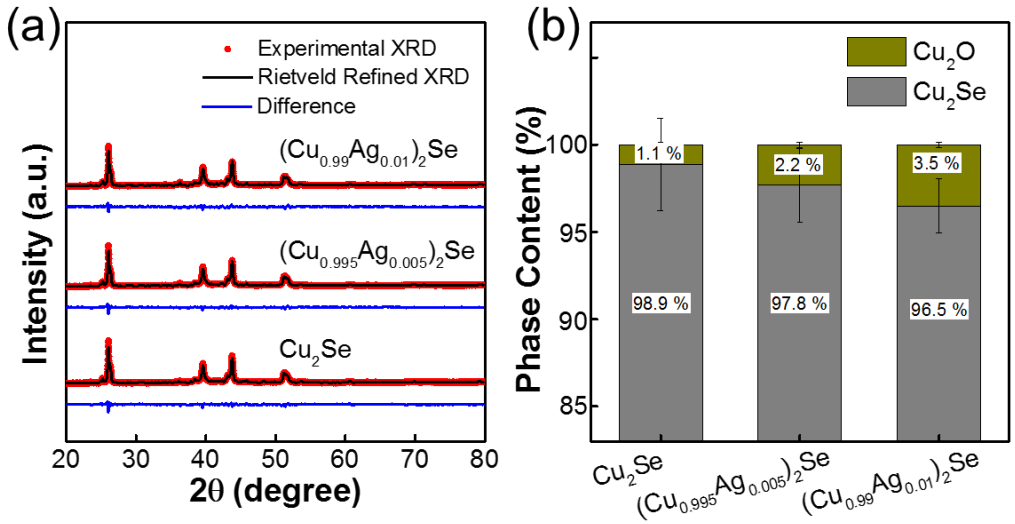

Figure S1. (a) Experimental and Rietveld refinement calculated XRD patterns and (b) Rietveld refinement calculated phase content of as-prepared Cu_2Se, $(Cu_{0.995}Ag_{0.005})_2Se$ and $(Cu_{0.99}Ag_{0.01})_2Se$ pellets.

2. Temperature-dependent specific heat of as-prepared $(Cu_{1-x}Ag_x)_2Se$ pellets

The temperature-dependent specific heat (C_p) of as-prepared $(Cu_{1-x}Ag_x)_2Se$ pellets are shown in Figure S2 (refer to Figure R2). The peaks at ~400 K of all samples clearly revealed the well-known phase transition from α-Cu_2Se to β-Cu_2Se at ~400 K.[2, 3] Here, we are mainly focusing on thermoelectric performance of $(Cu_{1-x}Ag_x)_2Se$ pellets after the phase transition where the temperature is higher than 423 K.

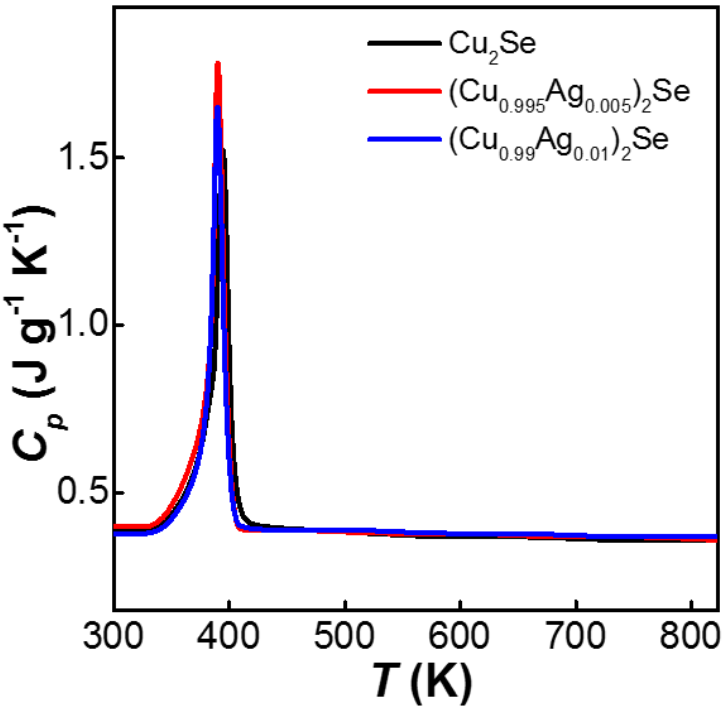

Figure S2. Temperature (T)-dependent specific heat (C_p) of as-prepared $(Cu_{1-x}Ag_x)_2Se$ pellets.

Reference

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