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Electronic Supporting Information (ESI)

Enhanced Thermoelectric Performance in *p*-type $AgSbSe_2$ by Cd-Doping †

Satya N. Guin,[a¥] Arindom Chatterjee[a¥] and Kanishka Biswas[a*]

[a]*New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bangalore- 560 064, India*

**E-mail: kanishka@jncasr.ac.in*

[¥]These two authors contributed equally

Experimental Section:

Materials. The following elements were used for the synthesis without further purification. Elemental silver (Ag, 99.9%, metal basis, Alfa Aesar), elemental antimony (Sb, 99.9999%, metal basis, Alfa Aesar), elemental cadmium (Cd, 99.9 %, Sigma Aldrich), elemental selenium (Se, 99.999%, metal basis, Alfa Aesar).

Synthesis. Ingots (~9 g) of $AgSb_{1-x}Cd_xSe_2$ (x = 0-6 mol%) were synthesized by mixing appropriate ratios of high-purity elemental Ag, Sb, Cd and Se in quartz tube. The tubes were sealed under vacuum (~10^{-5} Torr) and slowly heated up to 673 K over 12 h, then heated up to 1123 K in 4h, soaked for 10 h, and subsequently air quenched to room temperature. For electrical and thermal transport measurements, the samples were cut and polished in presence of water. In Figure 1(a), we show a photograph of "as synthesized" high quality ingot of $AgSb_{0.98}Cd_{0.02}Se_2$. Bar-shaped samples were used for simultaneous electrical conductivity and Seebeck coefficient measurement and coin-shaped samples were used for thermal conductivity measurement.

Powder X-ray diffraction. Powder X-ray diffraction for all the samples were recorded on a Bruker D8 diffractometer using a Cu K_α (λ = 1.5406 Å) radiation.

Thermoelectric measurements. σ and S were measured simultaneously using 2 mm ×3 mm ×8 mm, dimension sample using a ULVAC-RIKO ZEM-3 instrument under helium atmosphere over 290 K to 650 K temperature range. The longer direction of the sample coincides with the direction in which the thermal conductivity was measured. Carrier concentrations of the sample calculated using Hall coefficient measurements at room temperature in a PPMS system. Thermal diffusivity, D, was directly measured and heat capacity, C_p, was indirectly derived using standard sample (pyroceram) in the range 298–650 K by using laser flash diffusivity method in a Netzsch LFA-457 instrument at N_2 atmosphere (Figure S2, SI). Thin cylinders with 8 mm diameter and 2 mm thickness were used in this measurement. κ_{total} was estimated using the formula, $\kappa_{total} = DC_p\rho$, where ρ is the density of the sample, measured from sample dimension and mass. The density of the pellets obtained was in the range ~98 % of the theoretical density. Heating and cooling cycles give repeatable transport properties for a given sample.

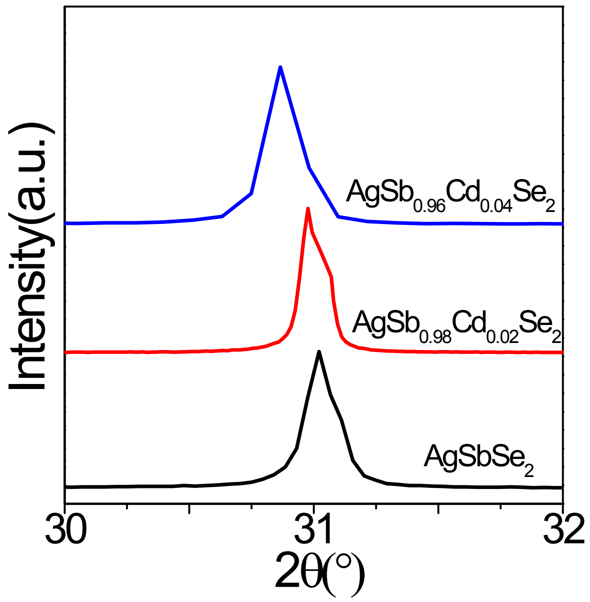

Fig. S1 Zoomed PXRD patterns of $AgSb_{1-x}Cd_xSe_2$ (x= 0-4 mol%) samples.

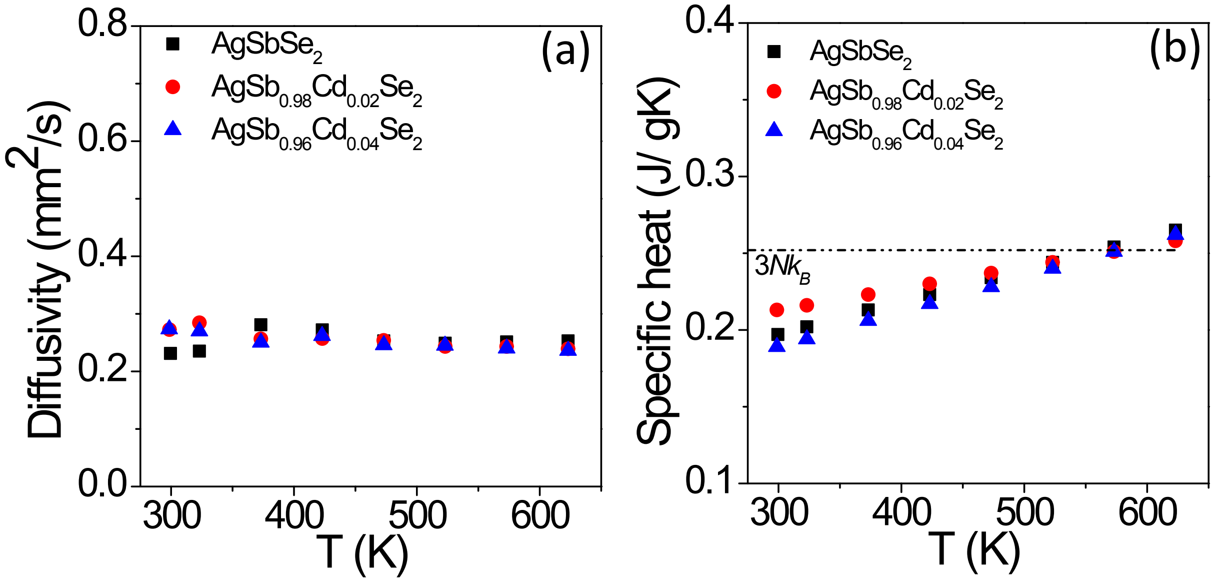

Fig. S2 Temperature dependent (a) thermal diffusivity and (b) specific heat of $AgSb_{1-x}Cd_xSe_2$ (x= 0-4 mol%) samples with Dulong–Petit specific heat at constant volume.