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

A low-temperature thermoelectric transport study of non-stoichiometric $AgSbTe_2$

Chinnu V. Devan[1,4], Mahima M. Kurian[2], P. N. Santhosh[2], Manoj Raama Varma[3, 4, *]

Biswapriya Deb[1, 4, *]

[1]*Centre for Sustainable Energy Technology (C-SET), CSIR- National Institute for Interdisciplinary Science and Technology (NIIST), Thiruvananthapuram- 695019, Kerala, India*

[2]*Department of Physics, Indian Institute of Technology Madras (IITM), Chennai 600036, India*

[3]*Materials Science and Technology Division, CSIR- National Institute for Interdisciplinary Science and Technology (NIIST), Thiruvananthapuram- 695019, Kerala, India*

[4]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India*

*Corresponding authors

Email: manojraamavarma@gmail.com, biswapriya.deb@niist.res.in

Tel.: +91-471-2515478, +91-471-2515377

Fax: +91-471-2491712

Characterization techniques

The crystal structure of synthesized $AgSbTe_2$ was analysed by powder X-ray diffraction techniques (Empyrean 3, PANalatycal X-ray diffractometer) using Cu-Kα radiation with wavelength 1.5406Å in the 2θ range 20° — 90° with a step size of 0.005°. The XRD data was refined using the software GSAS2. The microstructure and local composition were investigated by scanning electron microscopy (Zeiss EVO 18 cryo-SEM, operating voltage of 15 kV)) and high-resolution transmission electron microscopy (HRTEM (FEI Tecnai F20, operated at 300 kV). The elemental mapping of the samples was done by TEM-EDS. The density of the pellets was measured using the Archimedes method and the Vickers microhardness of the material was calculated using Vickers Microhardness tester - Banbros. The low temperature electrical and thermal transport measurements and heat capacity of the samples were done through the electrical transport option (ETO), thermal transport option (TTO, with ± 5% accuracy of thermal

conductance and Seebeck coefficient, 0.01 % for resistivity) and heat capacity set-up of physical property measurement system (PPMS, Quantum Design).

Table 1. Elemental weight percentage of $AgSbTe_2$ calculated and obtained from SEM-EDX

Element	Actual weight %	Average weight %
Ag	22.24	20.61
Sb	25.11	26.86
Te	52.63	52.76

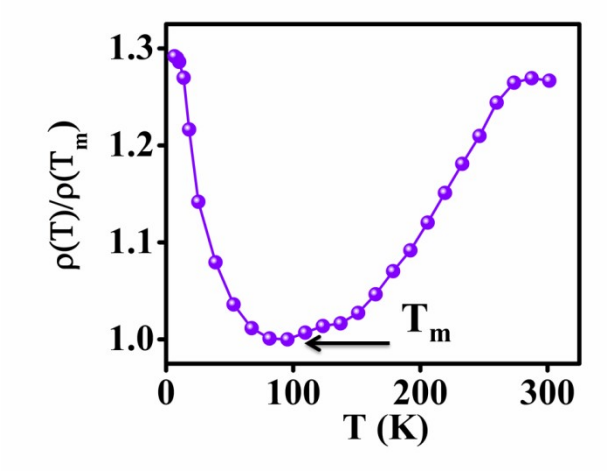

Figure S1. Normalized resistivity data versus T

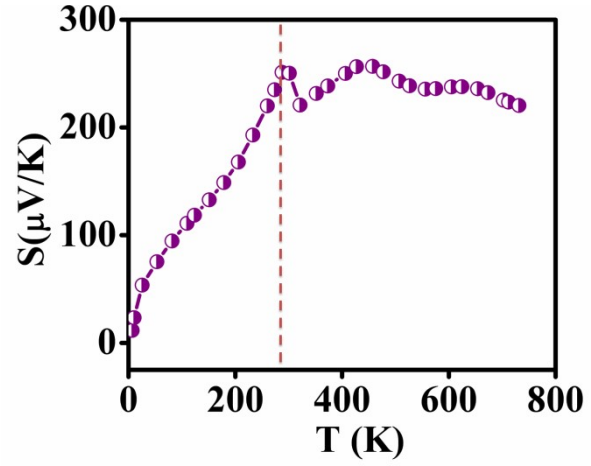

Figure S2. Variation of S with T

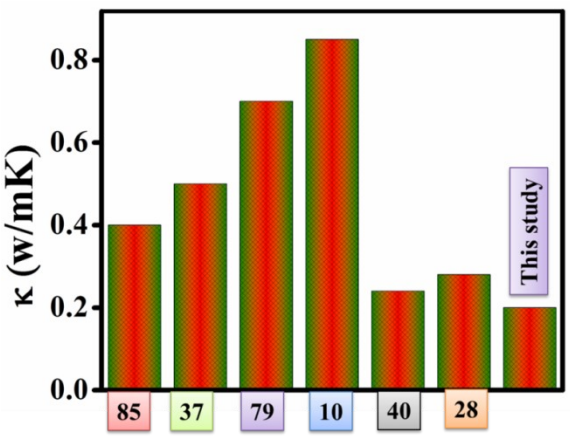

Figure S3. A comparison study on the thermal conductivity of the present material with previous reports

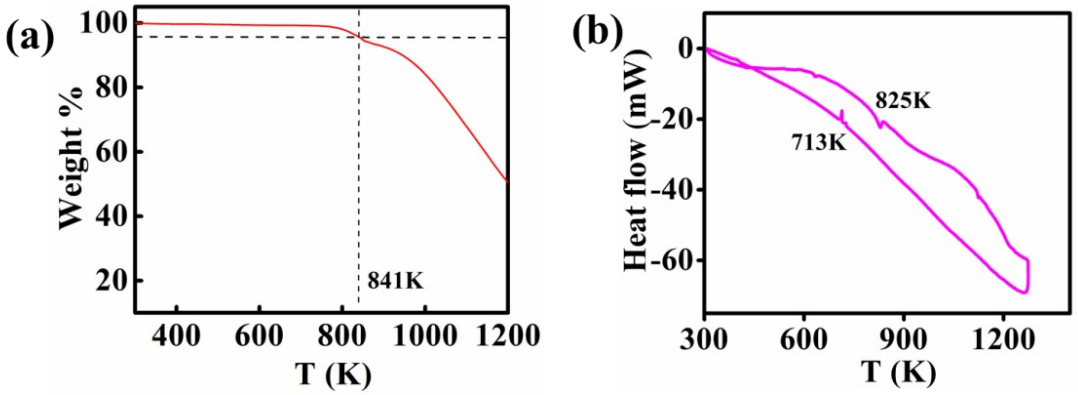

Figure S4. TGA and DTA of the material

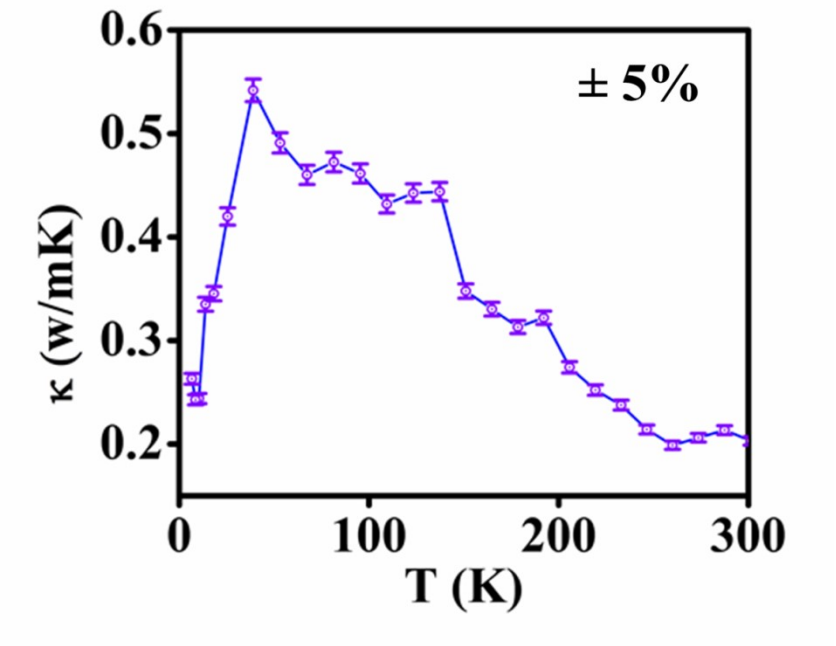

Figure S5 a: Plot of measured thermal conductivity versus temperature with error bar of ± 5%

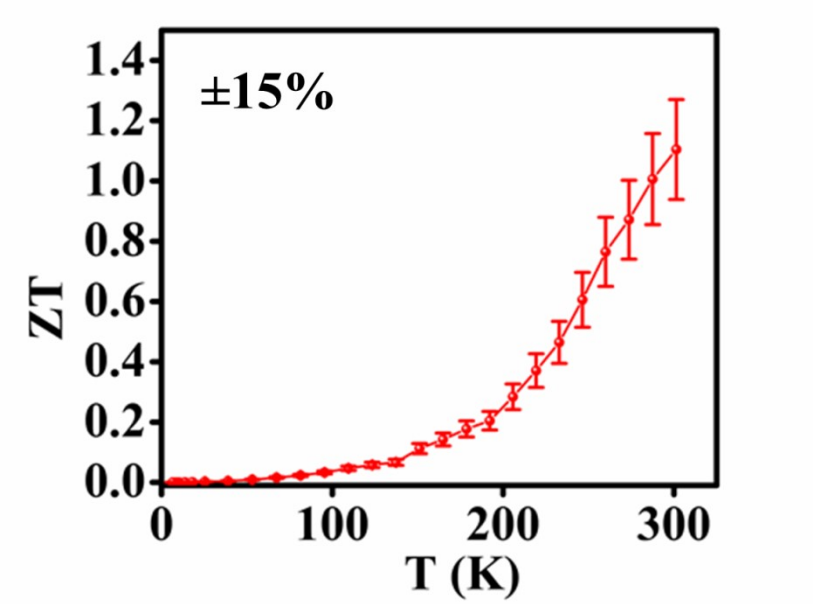

Figure S5 b: Plot of measured figure of merit versus temperature with error bar of ± 15%