Supporting Information

A Facile Surfactant-Assisted Reflux Method for the Synthesis of Single-Crystalline Sb_2Te_3 Nanostructures with Enhanced Thermoelectric Performance

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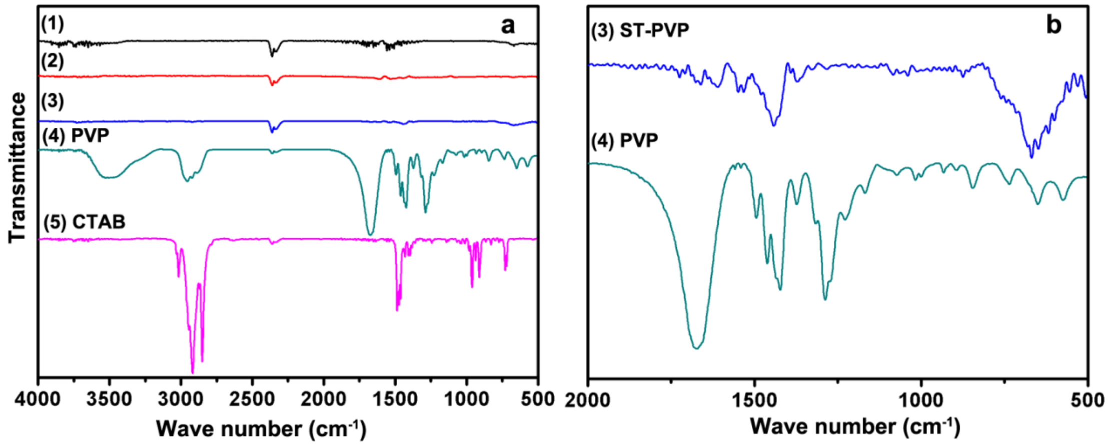

Fig. S1 FTIR spectra of the Sb_2Te_3 nanoparticles synthesized at 180 °C without or with surfactants. **a:** (1) without surfactant; (2) 8.0 g CTAB; (3) 0.6 g PVP; (4) pure PVP and (5) pure CTAB. **b:** magnification of FTIR spectra of (3) and (4) in the wave number of 500 ~ 2000 cm^{-1}.

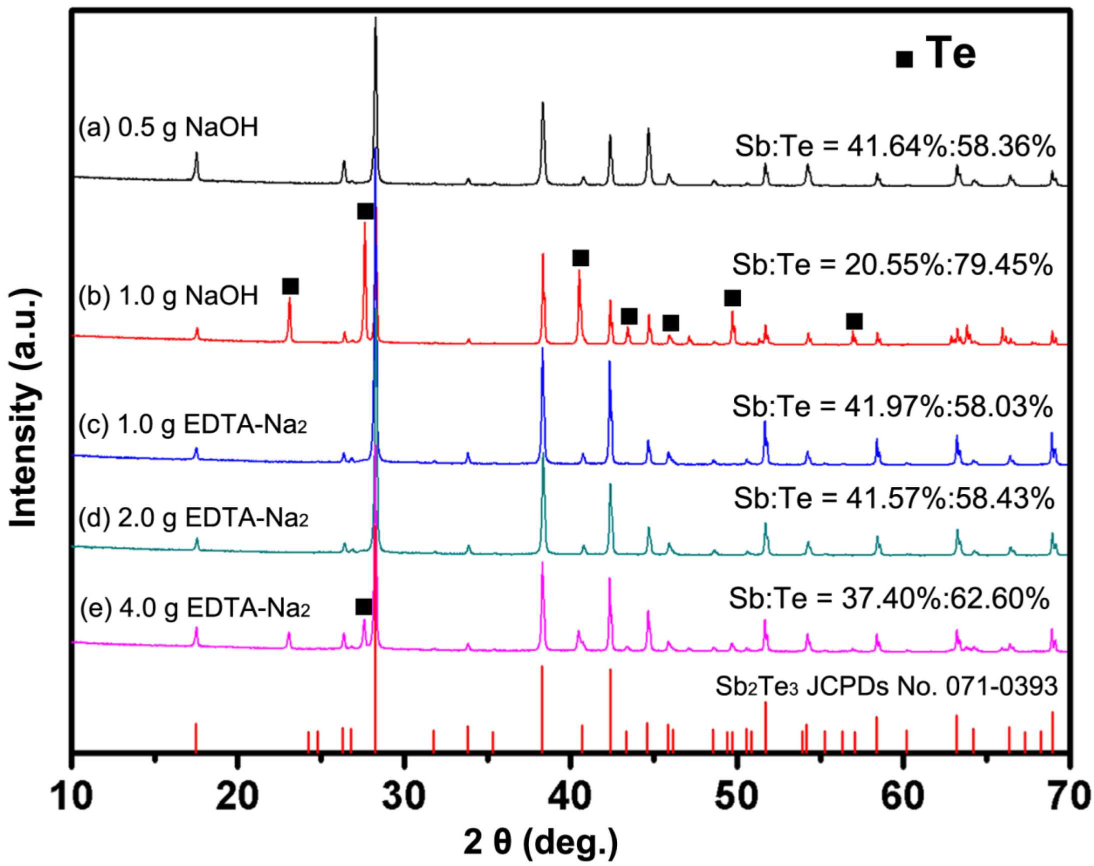

Fig. S2 XRD patterns of obtained Sb_2Te_3 nanoparticles in the presence of different inorganics and the list of atomic percent ratio of Sb:Te according to the corresponding EDS results. (a) 0.5 g NaOH; (b) 1.0 g NaOH; (c) 1.0 g EDTA-Na_2; (d) 2.0 g EDTA-Na_2; (e) 4.0 g EDTA-Na_2.

Calculation of the Lorentz number.

The Lorentz number is given as:

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

where $F_n(\eta)$ is the n-th order Fermi integral,

$$F_n(\eta) = \int_0^\infty \frac{x^n}{1+e^{x-\eta}} dx, \quad (2)$$

k_B is the Boltzmann constant, e is the electron charge, r is the scattering parameter, and η is the reduced Fermi energy, respectively. Let $r = -1/2$ by assuming that the acoustic phonon scattering is the dominant carrier scattering mechanism, then η could be derived from the measured Seebeck coefficient (S) by using the following relationship:

$$S = \pm \frac{k_B}{e} \left(\frac{\left(r+\frac{5}{2}\right)F_{r+\frac{3}{2}}(\eta)}{\left(r+\frac{3}{2}\right)F_{r+\frac{1}{2}}(\eta)} - \eta \right), \quad (3)$$

The The values of L at 50 °C are obtained 1.90×10^{-8}, 1.89×10^{-8}, 1.83×10^{-8} V^2K^{-2} for ST-CTAB, ST-0, ST-PVP, respectively.

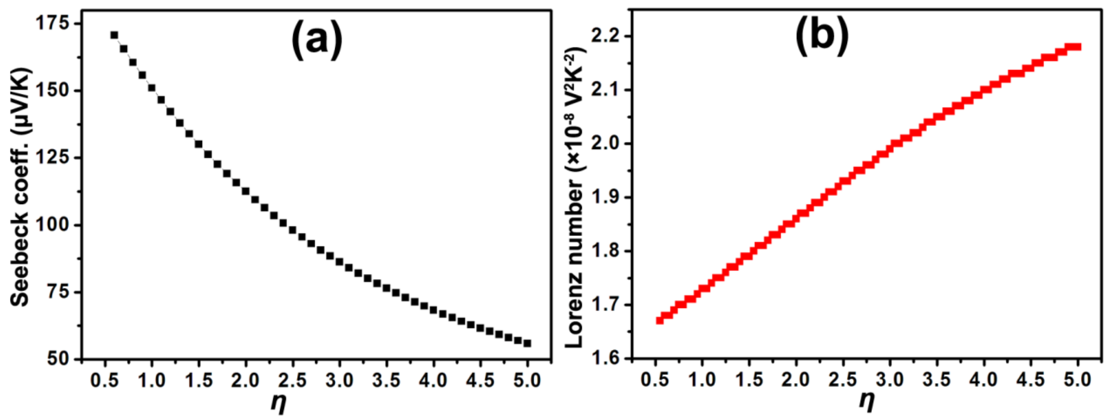

Fig. S3 The calculated relationships between the Seebeck coefficient, Lorentz number and reduced Fermi energy. (a) S ~ η; (b) L ~ η.