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

Designing and characterization of novel polymorphs of single-layered Tin-Sulfide for direction-dependent thermoelectric applications using first-principles approaches

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The SnS monolayers particularly the α-SnS, γ-SnS, and ε-SnS possess a high degree of anisotropy in structures. The estimated structural anisotropy in α-SnS, β-SnS, γ-SnS, δ-SnS, and ε-SnS magnitude 0.098, 0, 0.24, 0.007, and 0.36 respectively.

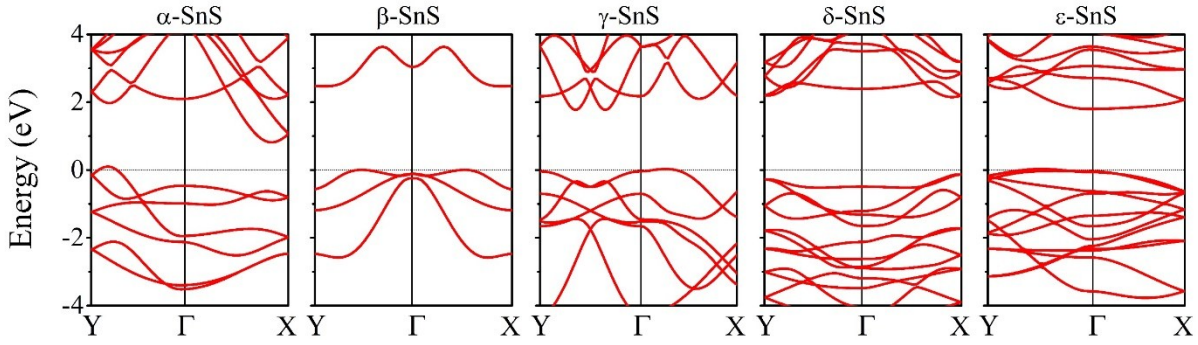

Figure S1. The electronic band structures determined with TB-mBJ potential along 100-direction (*x*- axis) and the 010-direction (*y*- axis) for α-, β-, γ-, δ- and ε- types of SnS monolayer.

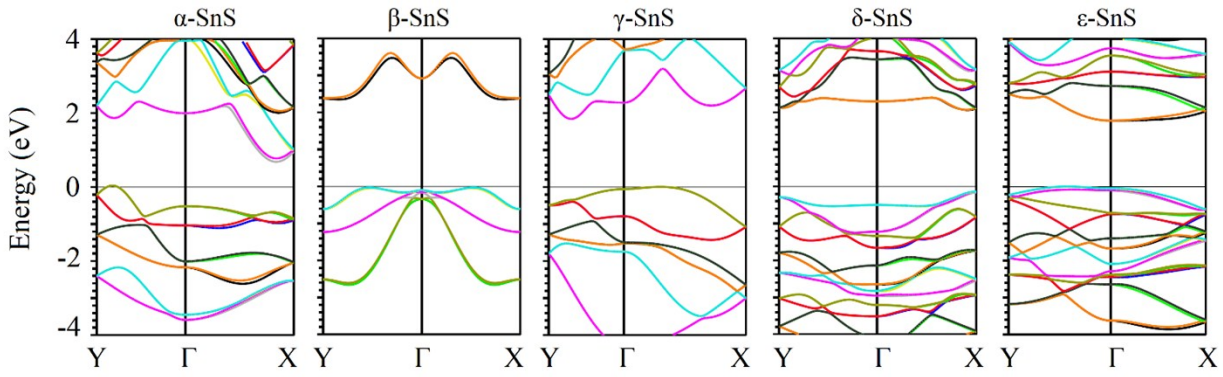

Figure S2. The electronic band structures determined with TB-mBJ+SOC along 100-direction (*x*-axis) and the 010-direction (*y*- axis) for α-, β-, γ-, δ- and ε- types of SnS monolayer.

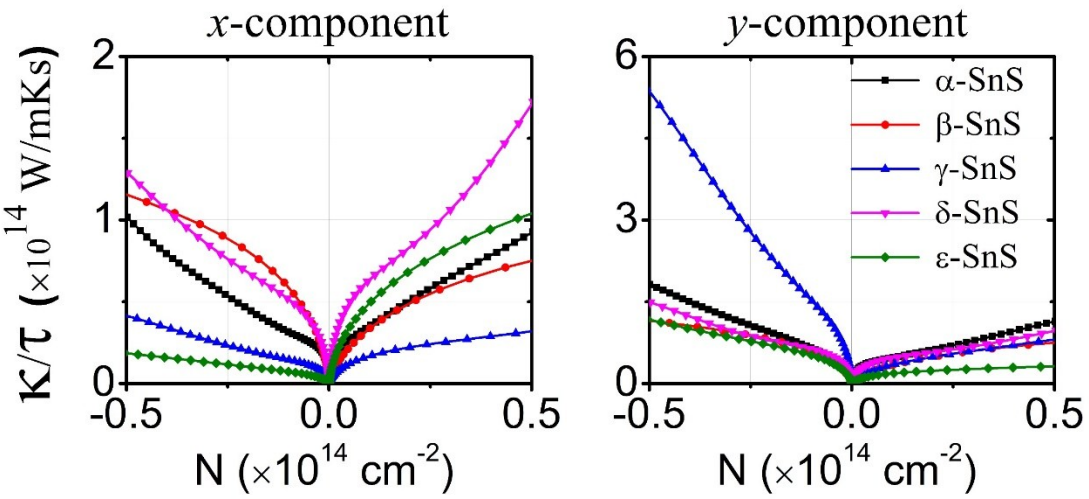

Figure S3. The dependence of *x*- and *y*- components thermal conductivity with respect to relaxation time ($\boldsymbol{\kappa}/\tau$) of SnS monolayers on the carrier's concentration