Supporting Information

Enhanced out-of-plane electrical transport in n-type SnSe thermoelectrics induced by resonant states and charge delocalization

Hulei Yu,[†,‡] Abdul Rehman Shaikh,[†] Fen Xiong,[†,‡] and Yue Chen[*,†,‡]

†*Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China*

‡*HKU Zhejiang Institute of Research and Innovation, 1623 Dayuan Road, Lin An 311305, China*

E-mail: yuechen@hku.hk

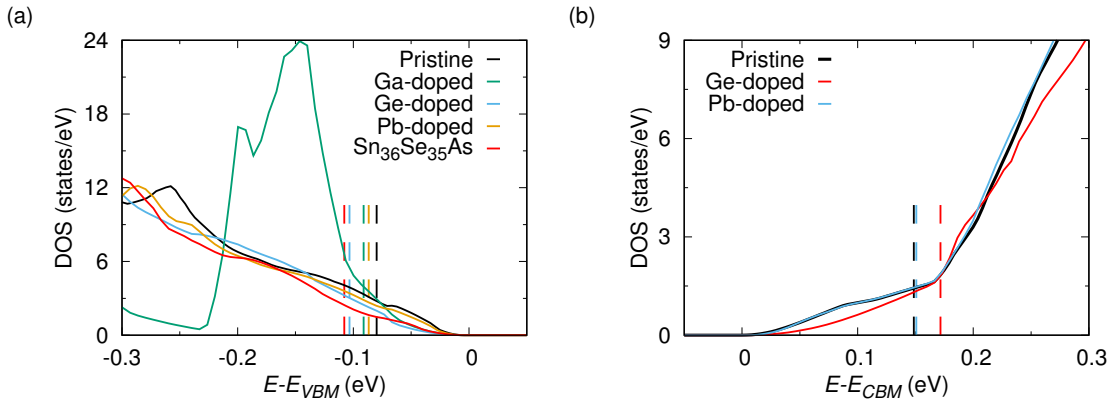

Figure S1: Density of states (DOS) of pristine and doped SnSe. (a) The valence band DOS. (b) The conduction band DOS. The vertical dashed lines represent the positions corresponding to a carrier concentration of 10^{20} cm^{-3}.

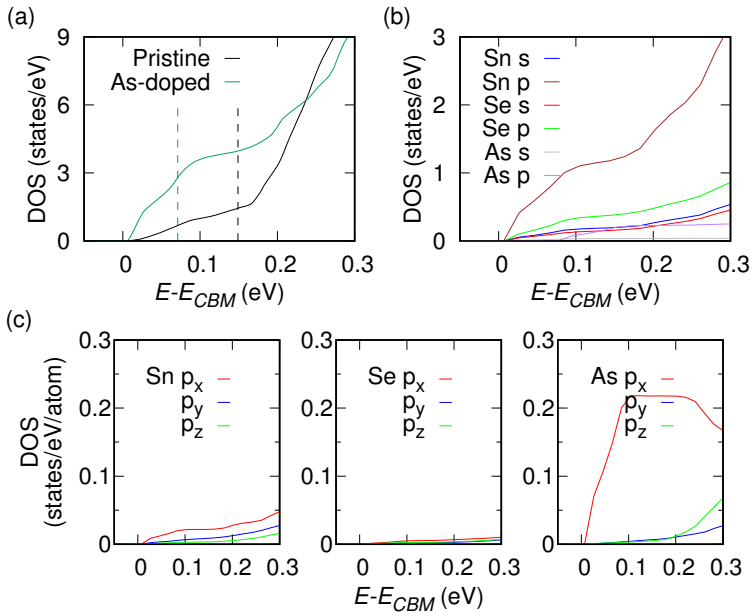

Figure S2: (a) Density of states of pristine and As-doped SnSe, where As substitutes for the Sn site. The vertical dashed lines represent the positions corresponding to a carrier concentration of 10^{20} cm^{-3}. (b and c) The projected DOS of As-doped SnSe.

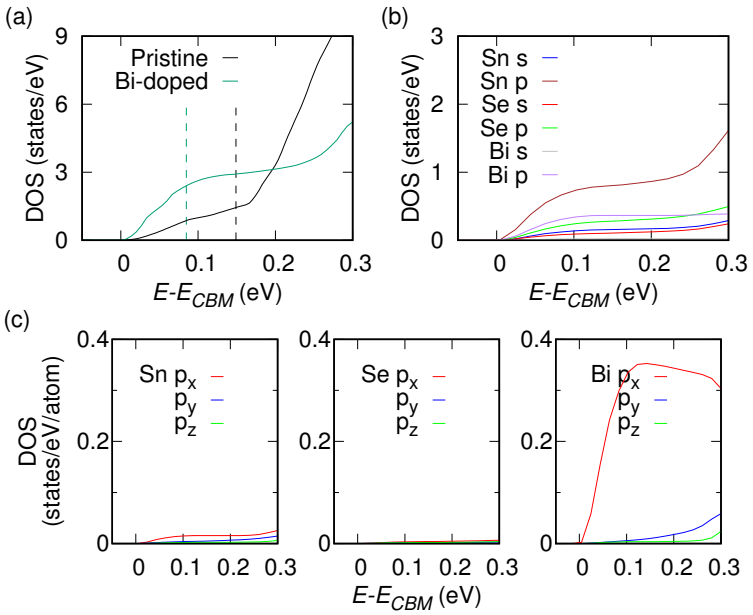

Figure S3: (a) Density of states of pristine and Bi-doped SnSe, where Bi substitutes for the Sn site. The vertical dashed lines represent the positions corresponding to a carrier concentration of 10^{20} cm^{-3}. (b and c) The projected DOS of Bi-doped SnSe.

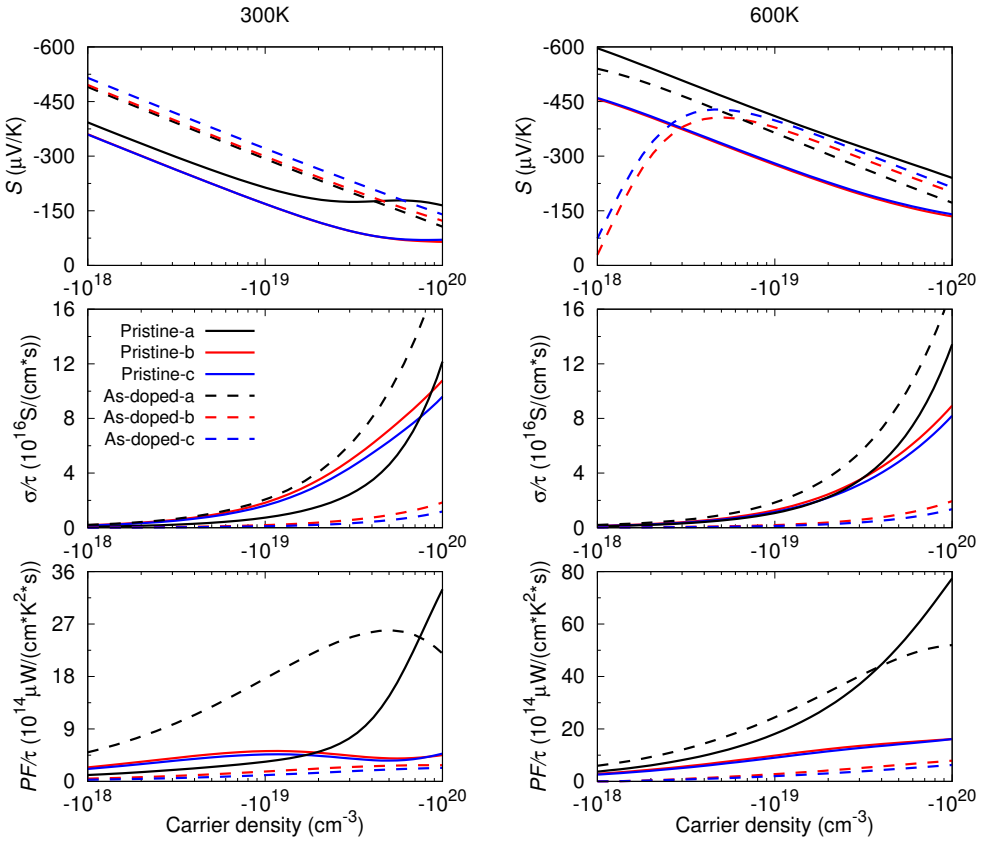

Figure S4: Seebeck coefficients (top), electrical conductivities normalized by the relaxation time (middle), and normalized power factors (bottom) of As-doped SnSe, where As substitutes for the Sn site.

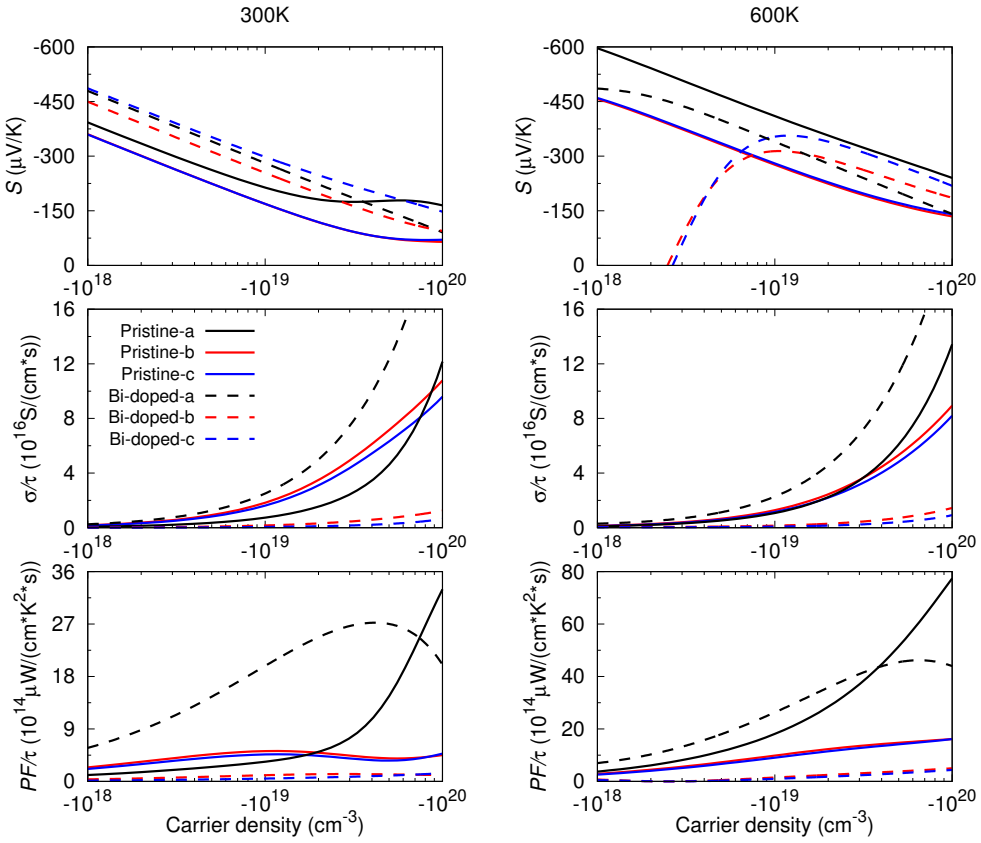

Figure S5: Seebeck coefficients (top), electrical conductivities normalized by the relaxation time (middle), and normalized power factors (bottom) of Bi-doped SnSe, where Bi substitutes for the Sn site.