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

Supplemental Information

The coexistence of superior intrinsic piezoelectricity and thermoelectricity in two-dimensional Janus α-TeSSe

Shaobo Chen, [ab] Xiangrong Chen, [a] Zhaoyi Zeng, *[c] Huayun Geng, [d] Huabing Yin, *[e]

[a] College of Physics, Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, P.R. China;

[b] College of Electronic and Information Engineering, Anshun University, Anshun 561000, P.R. China;

[c] College of Physics and Electronic Engineering, Chongqing Normal University, Chongqing 400047, P.R. China;

[d] National Key Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, CAEP, Mianyang 621900, P.R. China

[e] Institute for Computational Materials Science, School of Physics and Electronics, International Joint Research Laboratory of New Energy Materials and Devices of Henan Province, Henan University, Kaifeng 475004, P.R. China

* Corresponding author. Email: zhaoyizeng@126.com; yhb@henu.edu.cn

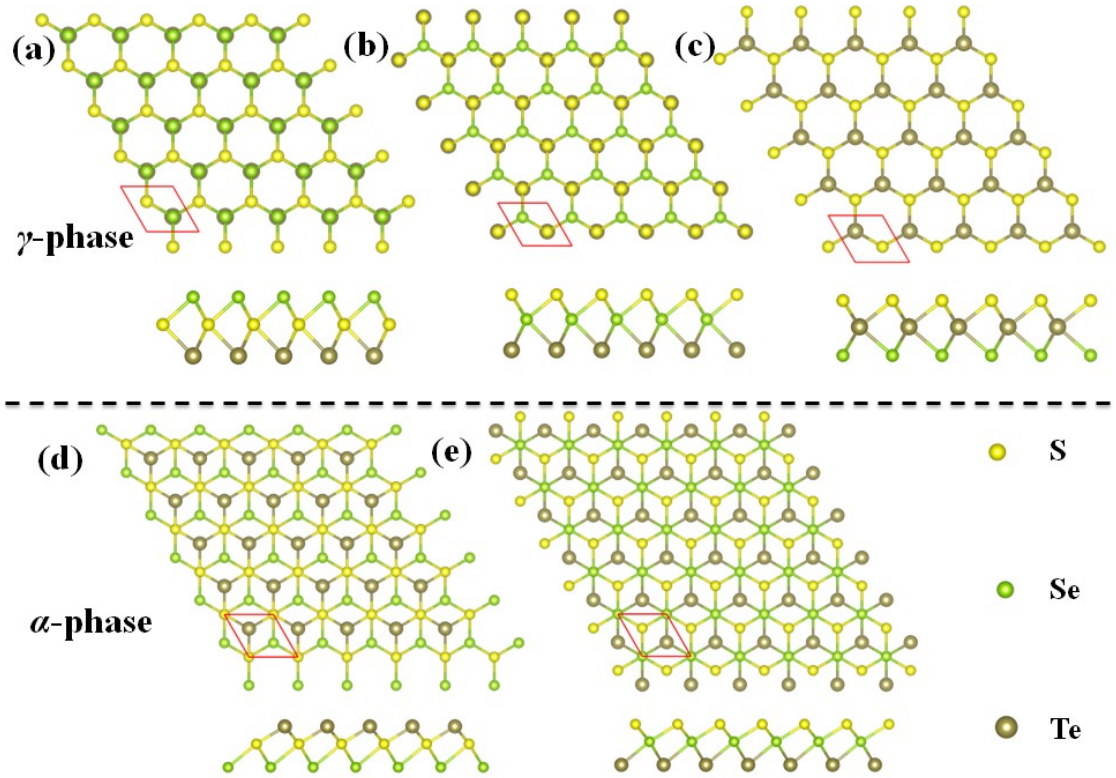

Fig. S1 (Color online) The structures of γ-phase and α-phase group-VI Janus compounds: (a) γ-SSeTe, (b) γ-SeSTe, (c) γ-TeSSe, (d) α-SSeTe, and (e) α-SeSTe. The red diamond wireframe represents the unit cell.

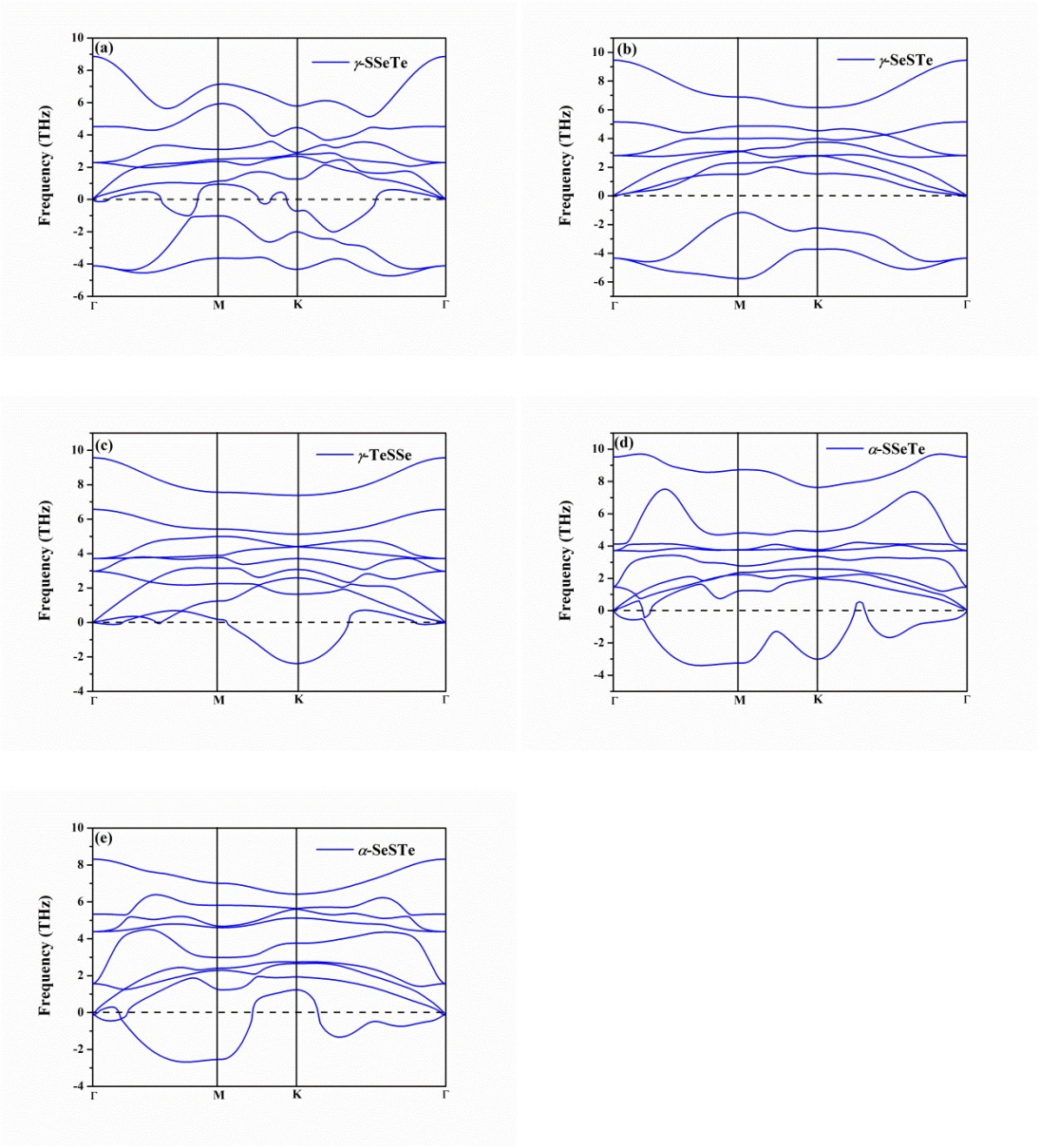

Fig. S2 (Color online) The phonon dispersion spectrum of Janus group-VI monolayers with γ-phase and α-phase corresponded to the structures in Fig. S1. A $5\times5\times1$ supercell is used to calculate the phonon frequency via the PHONOPY code.

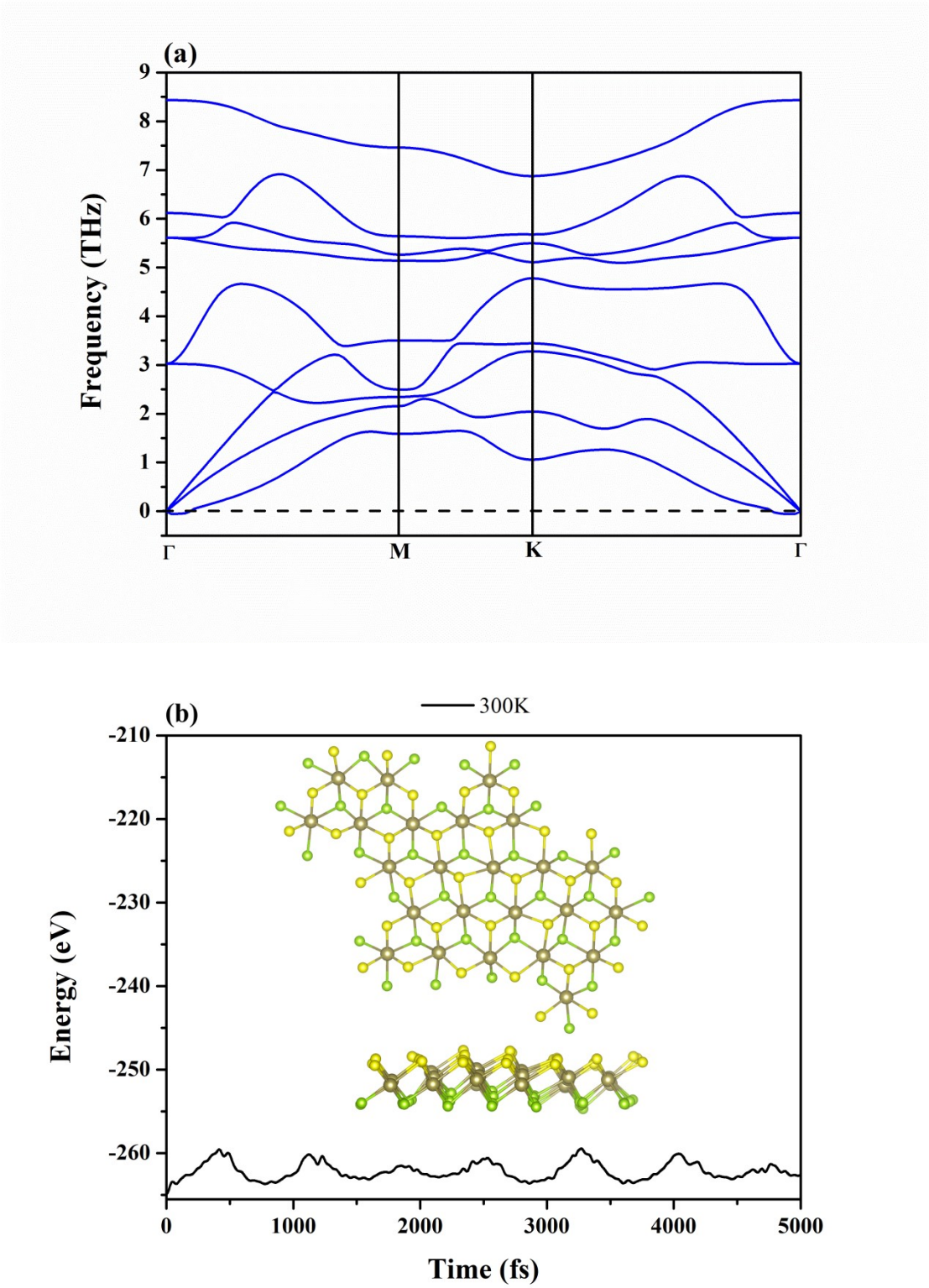

Fig. S3 (Color online) (a) Phonon spectrum and (b) ab initio molecular dynamics simulation of the Janus α-TeSSe monolayer.

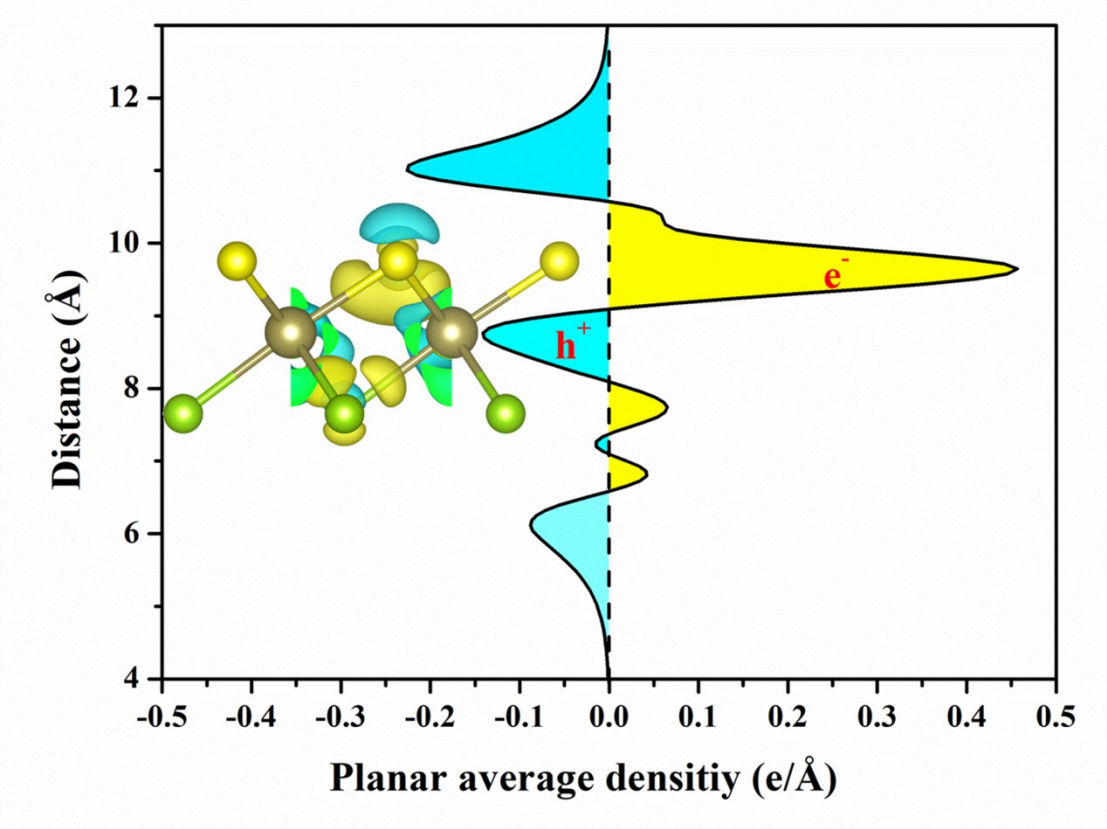

Fig. S4 (Color online) Charge density difference and the planar averaged charge density difference of α-TeSSe monolayer along the z-direction. The light blue areas indicate the depletion of electrons and the yellow areas indicate the accumulation of electrons.

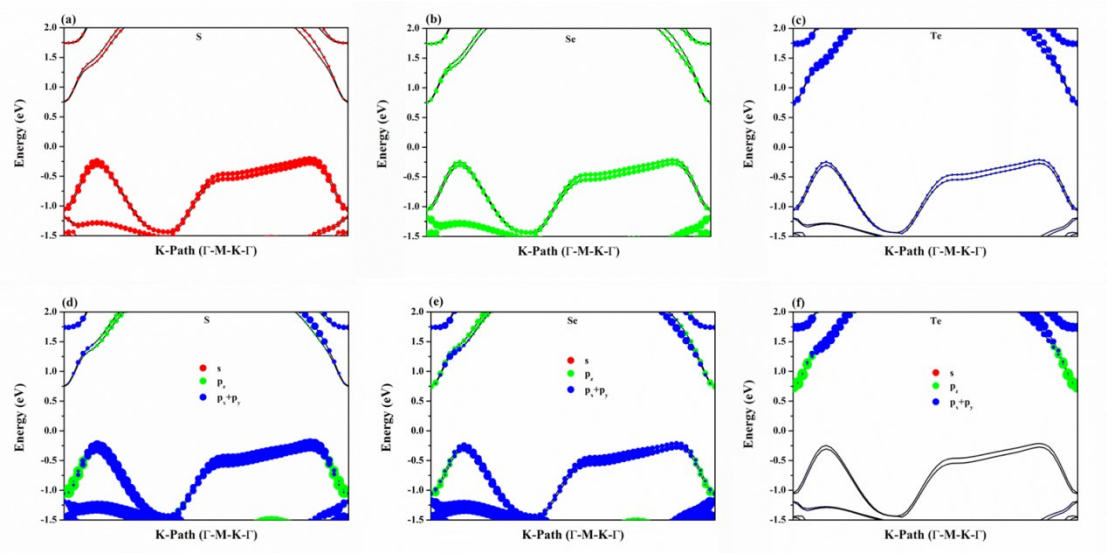

Fig. S5 (Color online) The (a-c) atom-projected and (d-f) orbital-projected band structures with SOC effect based on HSE06 functional for independent element S, Se, and Te, respectively. The radius of the circles represents the weight of each atom and orbital.

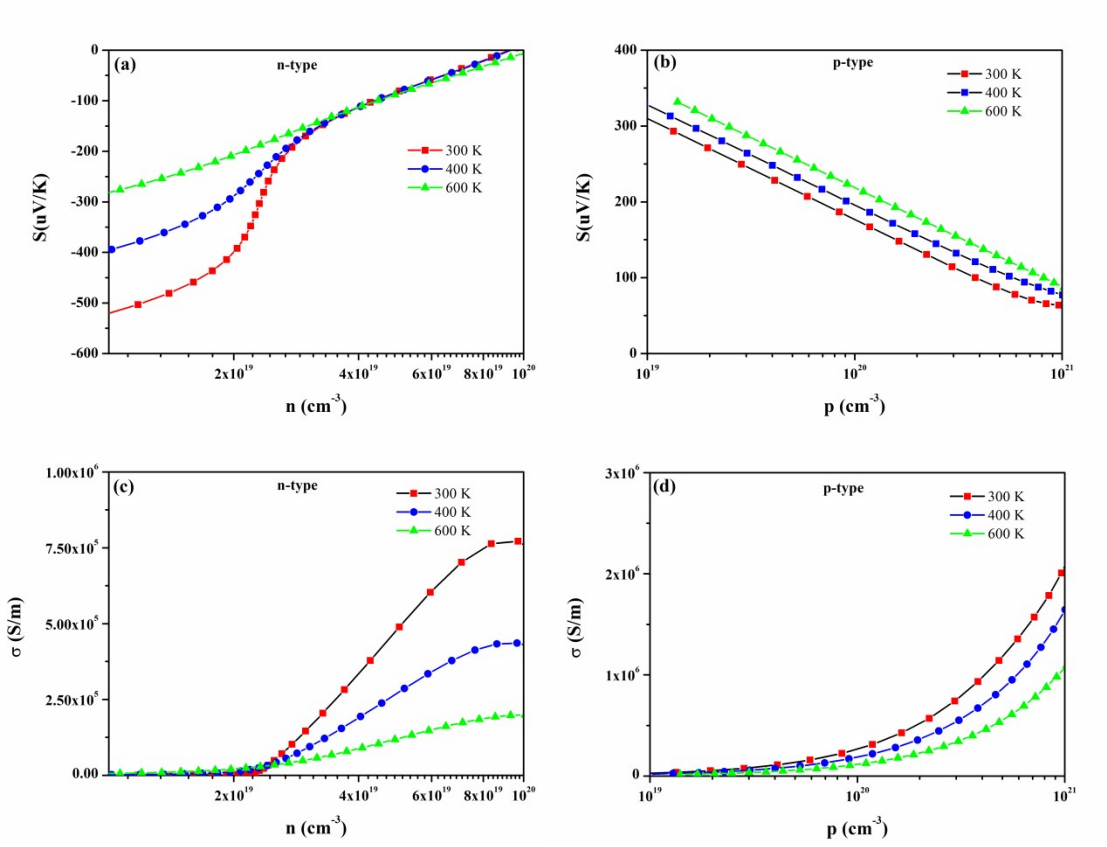

Fig. S6 (Color online) The calculated (a, b) Seebeck coefficients *S* and (c, d) electronic conductivity σ of Janus TeSSe monolayer at different temperatures as a function of doping levels.