Supporting Information

The thermoelectric properties of α-XP (X=Sb and Bi) monolayers from a first-principles calculation

Xin Liu [1], Dingbo Zhang [1], Yuanzheng Chen [1], Hui Wang [1], Hongyan Wang [1] and Yuxiang Ni [1 a)]

[1] School of Physical Science and Technology, Southwest Jiaotong University, Chengdu 610031, P. R. China.

*** Corresponding author.**

Yuxiang Ni

School of Physical Science and Technology, Southwest Jiaotong University, Chengdu 610031, P. R. China.

E-mail Address: yuxiang.ni@swjtu.edu.cn

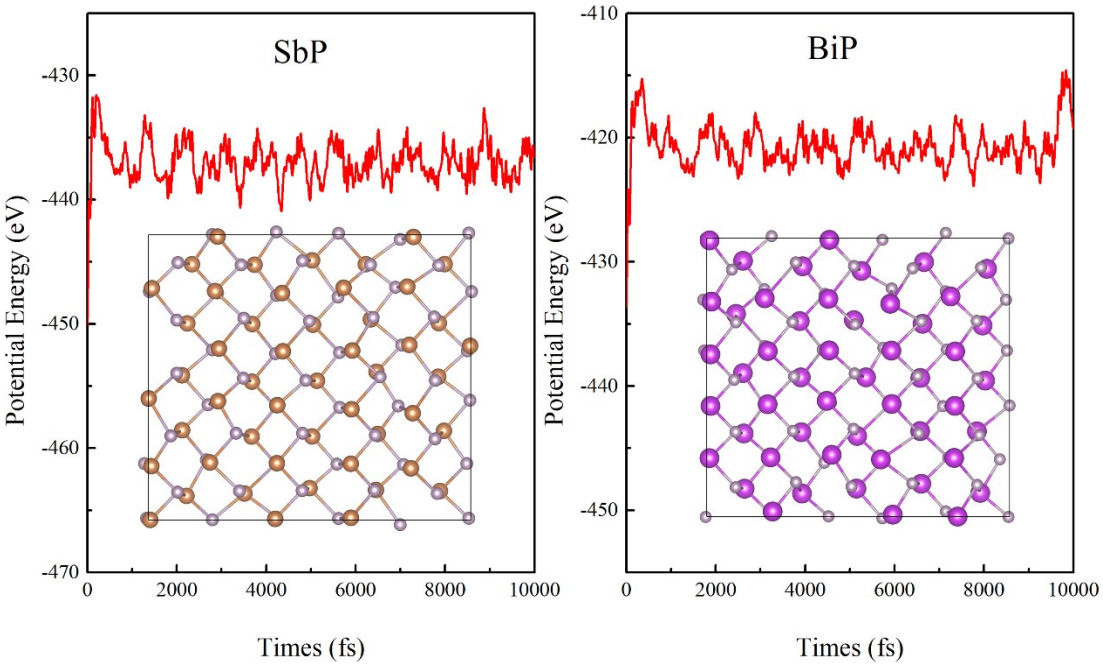

Fig. S1. The *ab initio* molecular dynamics (AIMD) simulations of time-dependent potential energy for α-SbP and α-BiP at 900 K.

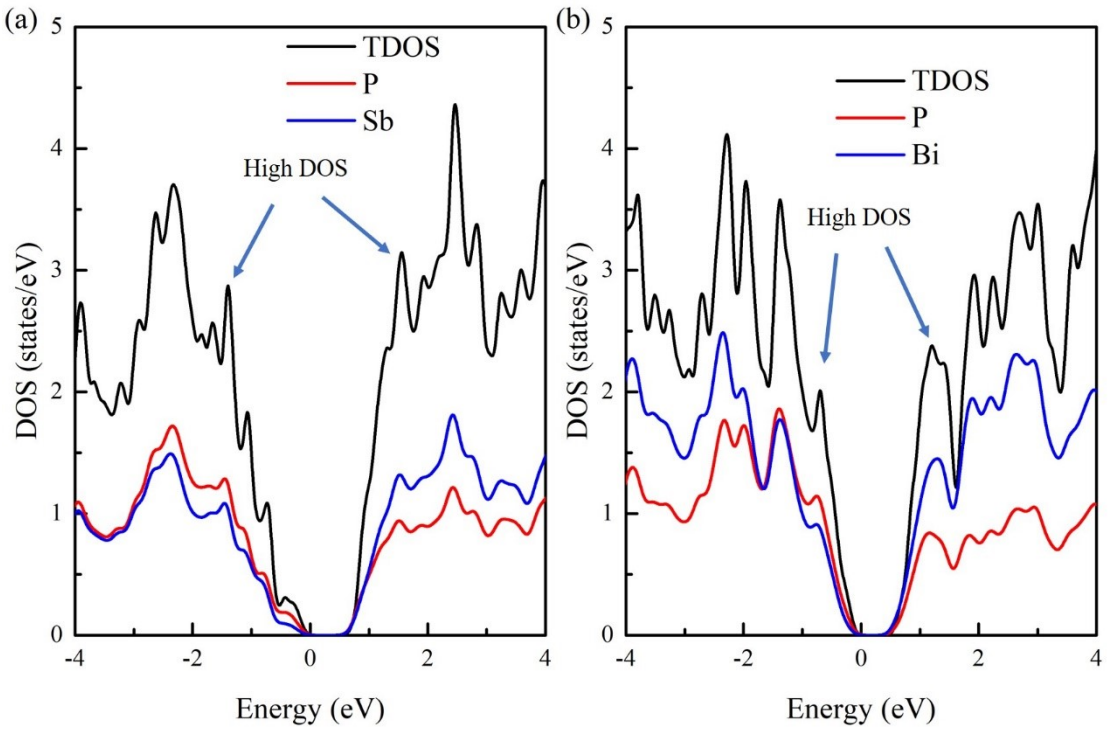

Fig. S2. The density of states (DOS) for SbP and BiP monolayers.

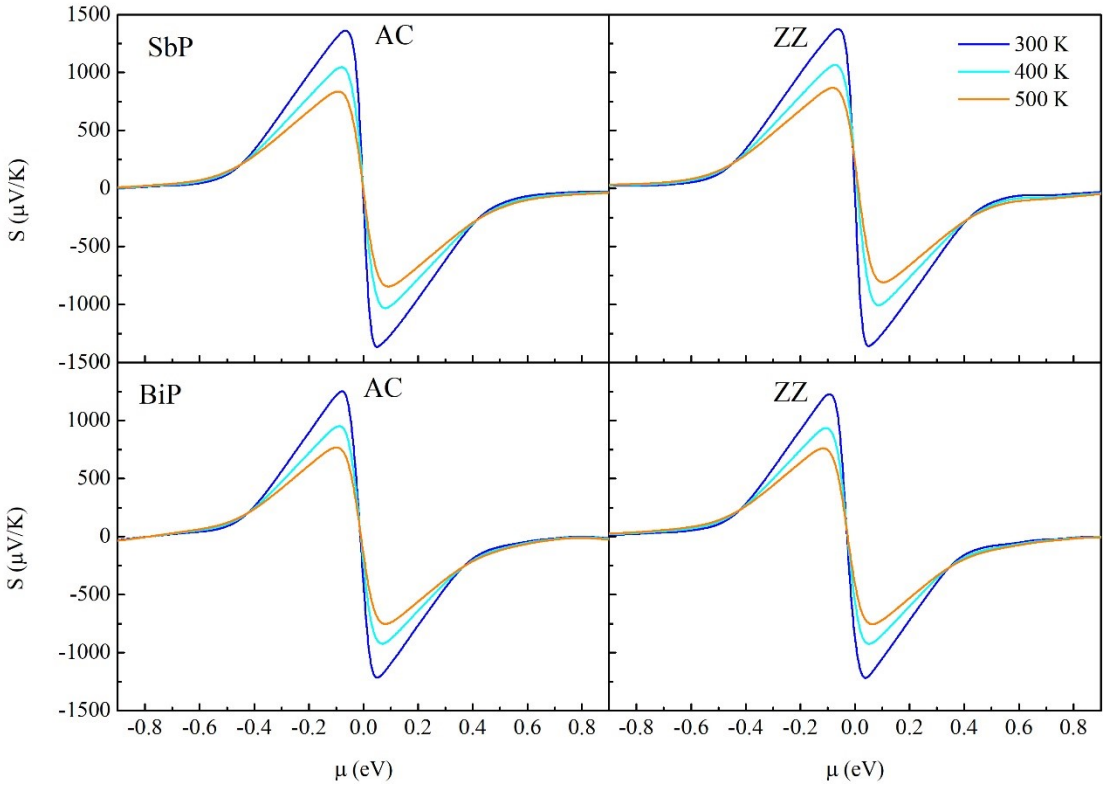

Fig. S3. Calculated Seebeck coefficient for SbP and BiP monolayers at 300 K, 400 K, and 500 K.

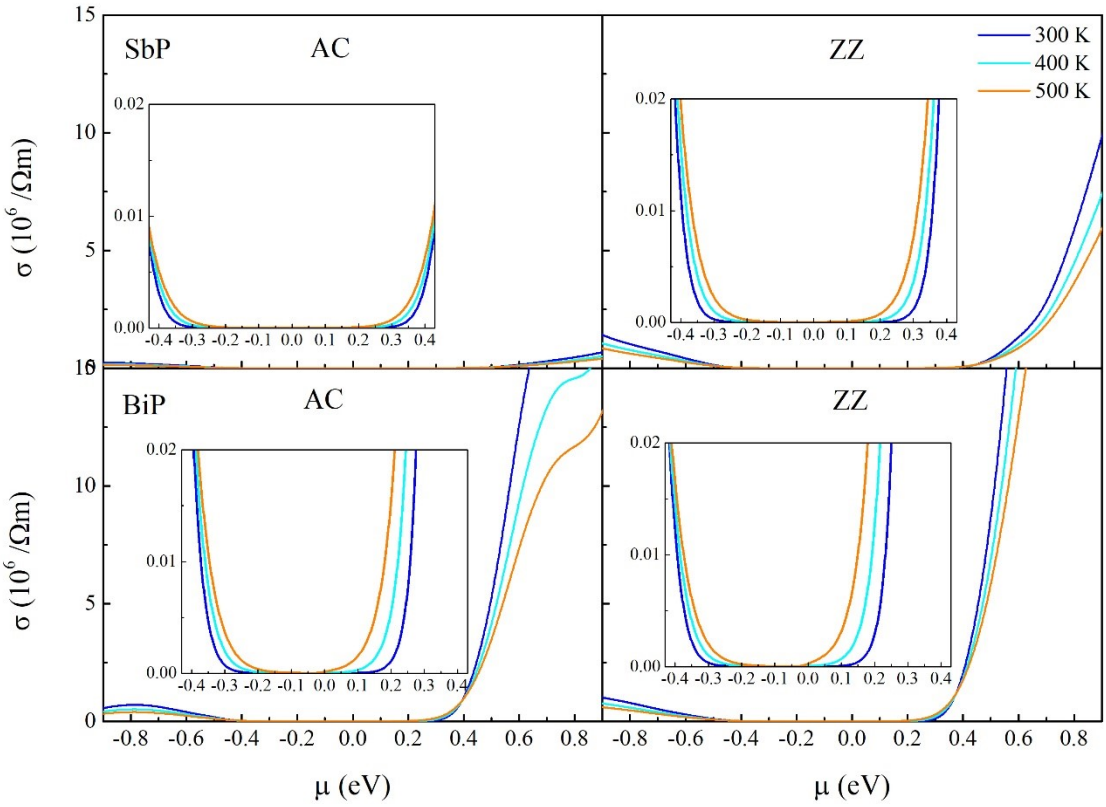

Fig. S4. Calculated electrical conductivity for SbP and BiP monolayers at 300 K, 400 K, and 500 K.

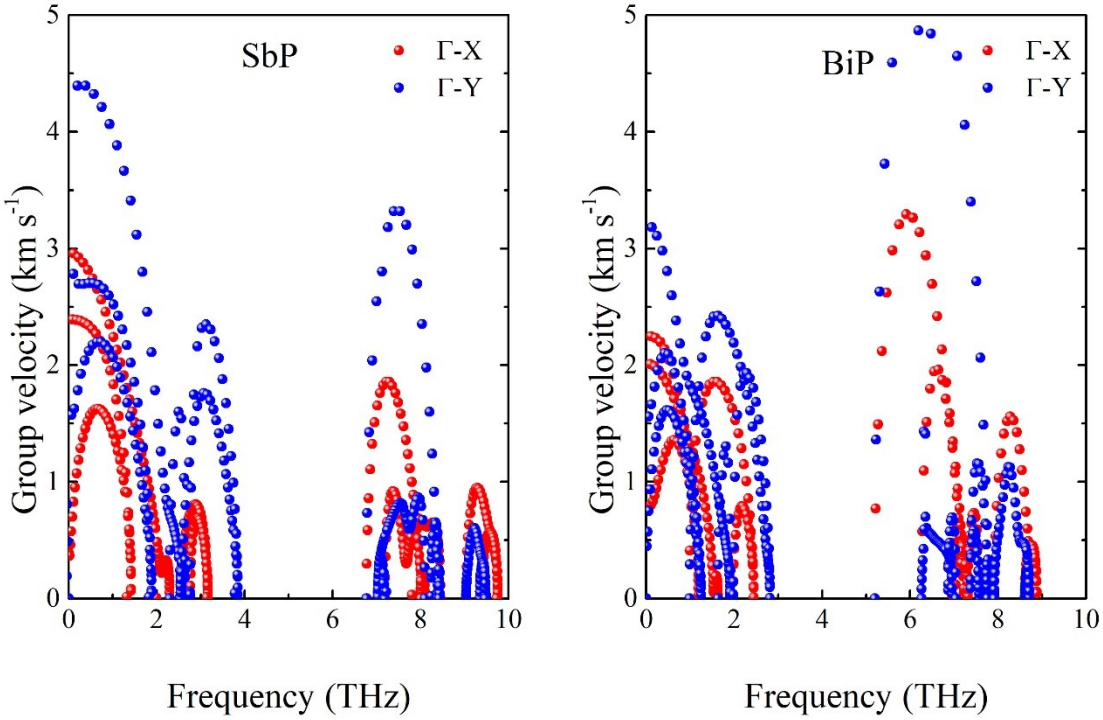

Fig. S5. The phonon group velocities along different highly symmetrical paths for SbP and BiP monolayers.

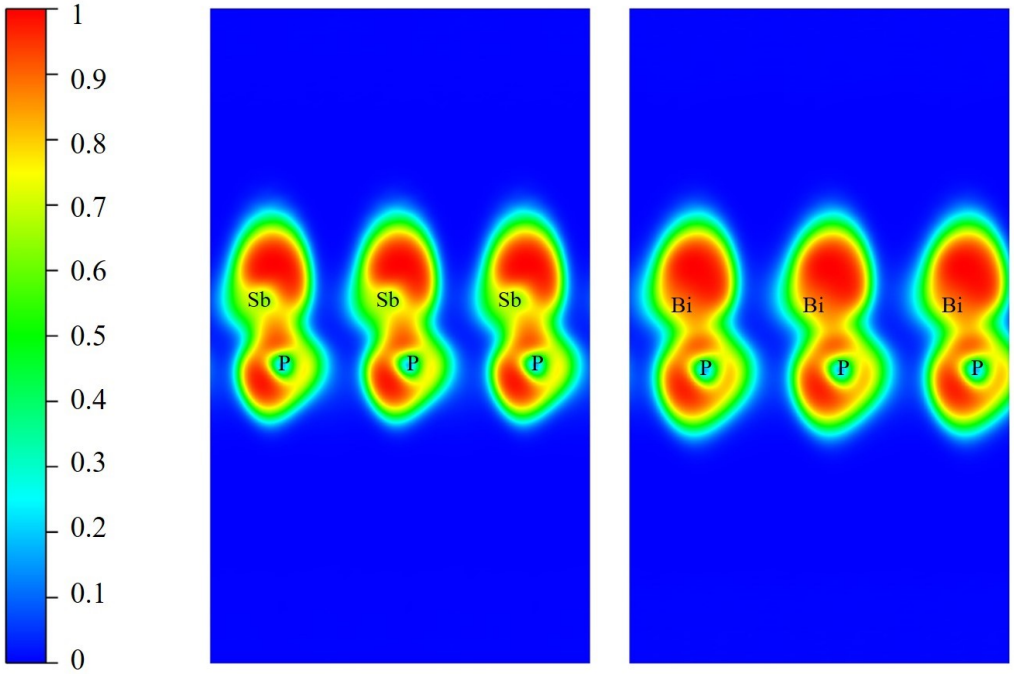

Fig. S6. The electronic localization function (ELF) for SbP and BiP monolayers.

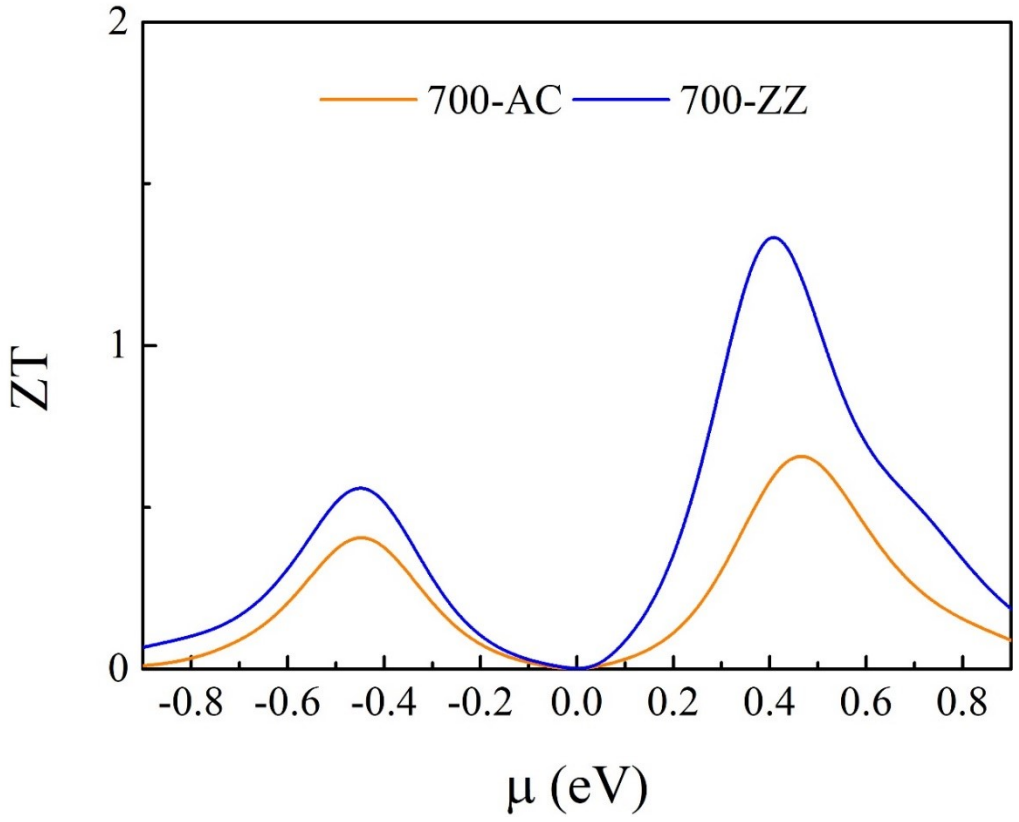

Fig. S7. Calculated figure of merit ZT for SbP monolayer at 700 K.

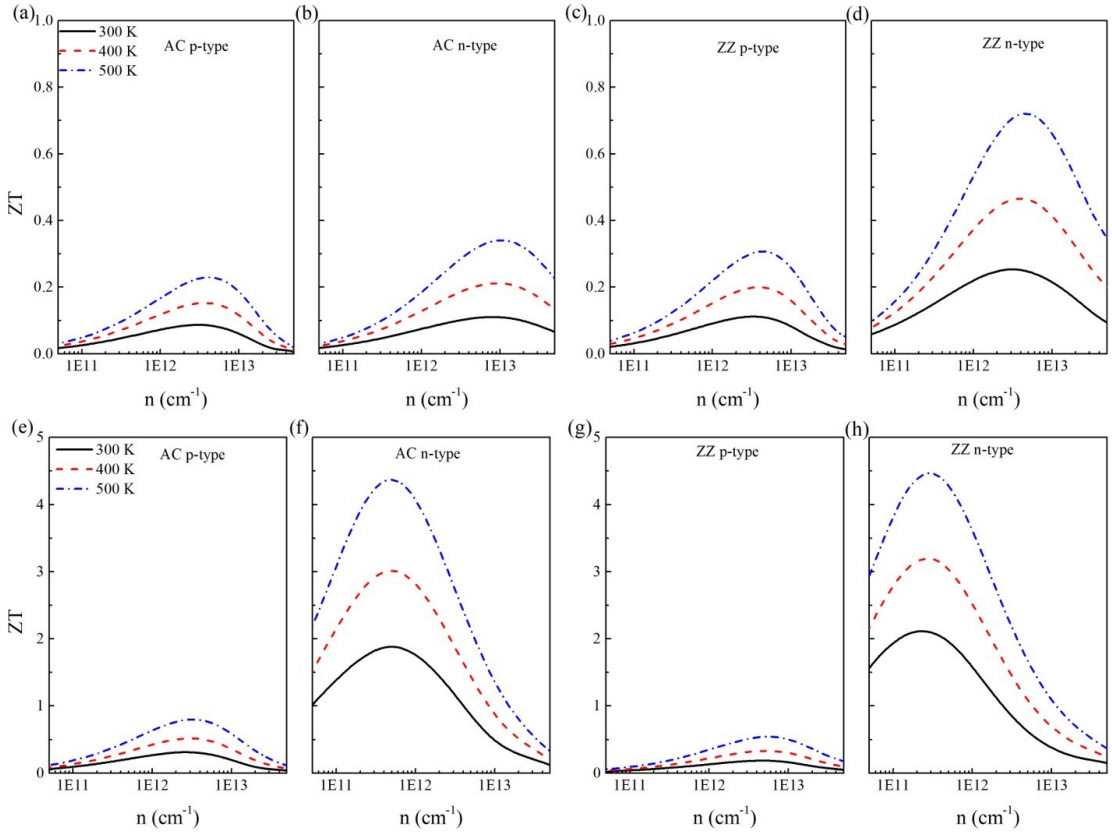

Fig. S8. The ZT values as a function of the doping concentration for the SbP monolayer and BiP monolayer.