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

"Supplementary Information"

Effects of biaxial tensile strain on the first-principles-driven thermal conductivity of buckled arsenene and phosphorene

Armin Taheri, Carlos Da Silva, Cristina H. Amon

(armin.taheri@mail.utoronto.ca)

Department of Mechanical and Industrial Engineering, University of Toronto, Ontario, Canada, M5S 3G8

1- Mechanical stability

To ensure the mechanical stability of the system, we check the Born criteria of the mechanical stability [1] . As can be seen from Figure 1, in the considered range of strain the elastic constants satisfy the following conditions:

$$C_{11} > 0,$$
$$C_{44} > 0,$$
$$C_{66} > 0,$$

which show that both β-As and β-P are mechanically stable for the whole range of strain considered in this work.

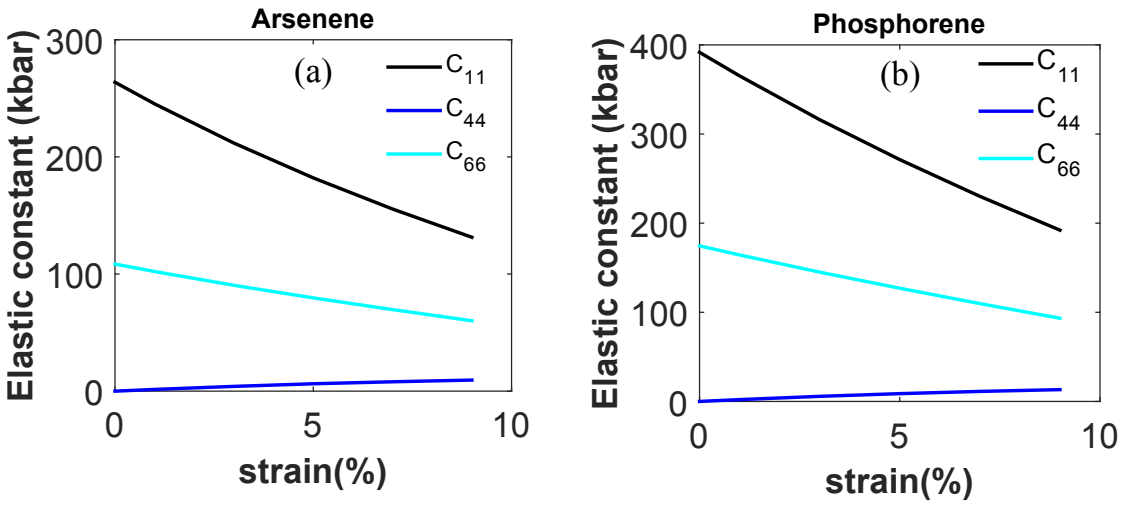

FIG. 1. Elastic constants of (a) arsenene, and (b) phosphorene under biaxial strain

1- Phonon dispersion convergence

Figure 2 shows the phonon dispersion curve of arsenene for two different phonon wave-vector grid of 7*7*1 and 9*9*1. One can see that a 7*7*1 is enough to have phonon dispersion converged.

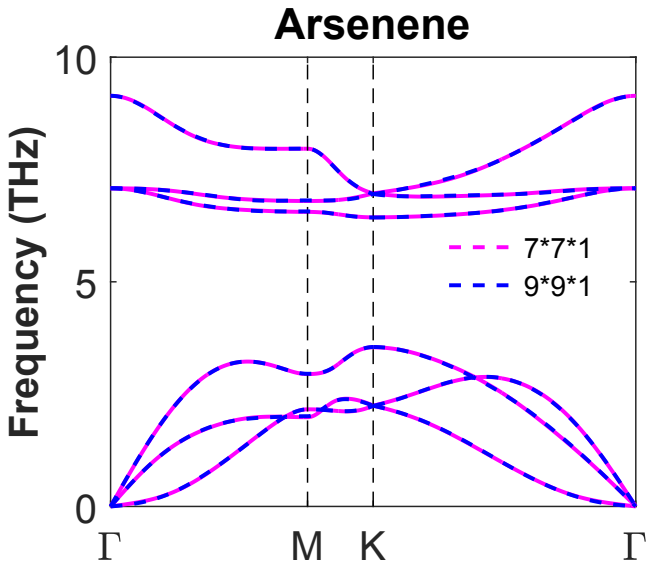

FIG. 2. Phonon dispersion convergence of arsenene with phonon wave-vector grid size

References

[1] Andrew R C, Mapasha R E, Ukpong A M and Chetty N 2012 Mechanical properties of graphene and boronitrene *Phys. Rev. B* **85** 125428