Supporting on-line Information for:

Tiling phosphorene

Jie Guan, Zhen Zhu, and David Tománek*

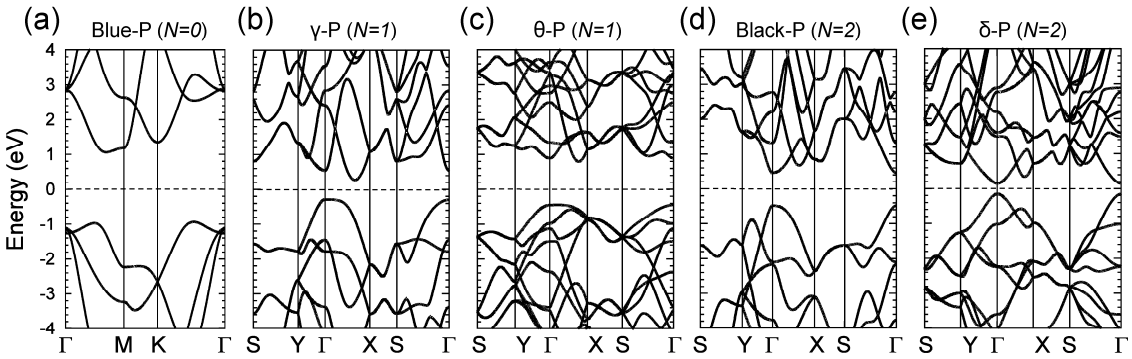

FIG. S1. Electronic band structure of (a) blue-P or β-P, (b) γ-P, (c) θ-P, (d) black-P or α-P, and (e) δ-P along high-symmetry lines.

ELECTRONIC BAND STRUCTURE OF DIFFERENT PHOSPHORENE ALLOTROPES

For the sake of completeness and better comparison, we have combined our band structure results for the different phosphorene allotropes in Fig. S1. Our results indicate that phosphorene allotropes of type *N=0* and *N=1*, shown in Figs. S1(a-c), have an indirect band gap. According to Figs. S1(d-e), *N=2* allotropes have a direct band gap.

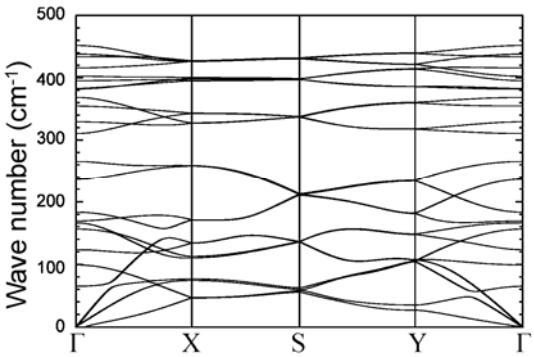

FIG. S2. Phonon band structure of θ-P along high-symmetry lines.

PHONON SPECTRA OF PHOSPHORENE ALLOTROPES

We have calculated the phonon spectrum of θ-P and present the phonon band structure in Fig. S2. We find the phonon spectrum of θ-P to be rather similar to previously published phonon spectra[1,2] of α-P, β-P, γ-P and δ-P. We found all these monolayer structures to be stable, as indicated by the absence of imaginary frequencies and soft phonon modes.

* tomanek@pa.msu.edu

1 Zhu, Z.; Tománek, D. Semiconducting Layered Blue Phosphorus: A Computational Study. *Phys. Rev. Lett.* **2014**, *112*, 176802.

2. Guan, J.; Zhu, Z.; Tománek, D. Phase Coexistence and Metal-Insulator Transition in Few-Layer Phosphorene: A Computational Study. *Phys. Rev. Lett.* **2014**, *113*, 046804.