Supplementary material

Tunable electronic and optoelectronic characteristics of two-dimensional β-AsP monlayer: A first-principles study

Zhong-Hui Xu,*[a,b,c,e] Kaiyu Wei,[a] Zhengyu Wang,[a] Junlin Jiang,[a] Guogang Liu[d] and San-Huang Ke [d]

[a] School of Information Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, China

[b] School of Science, Jiangxi University of Science and Technology, Ganzhou 341000, China

[c] Shanghai Key Laboratory of Special Artificial Microstructure Materials and Technology, Shanghai 200092, People's Republic of China

[d] MOE Key Laboratory of Microstructured Materials, School of Physics Science and Engineering, Tongji University, Shanghai 200092, China

[e] Jiangxi Province Key Laboratory of Multidimensional Intelligent Perception and Control, Ganzhou 341000, China

* Corresponding Author.

E-mail addresses: longxister@163.com

1. The electronic structures of monolayer *β*-AsP

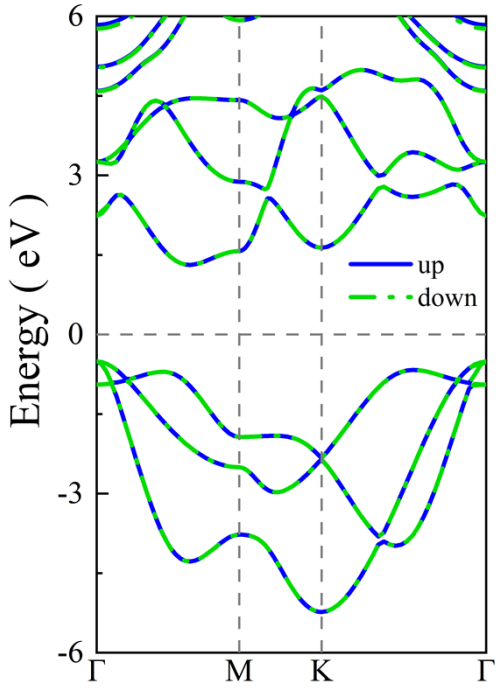

Fig. S1. Spin-polarized energy band structure of monolayer *β*-AsP.

2. The dynamic stability of monolayer *β*-AsP

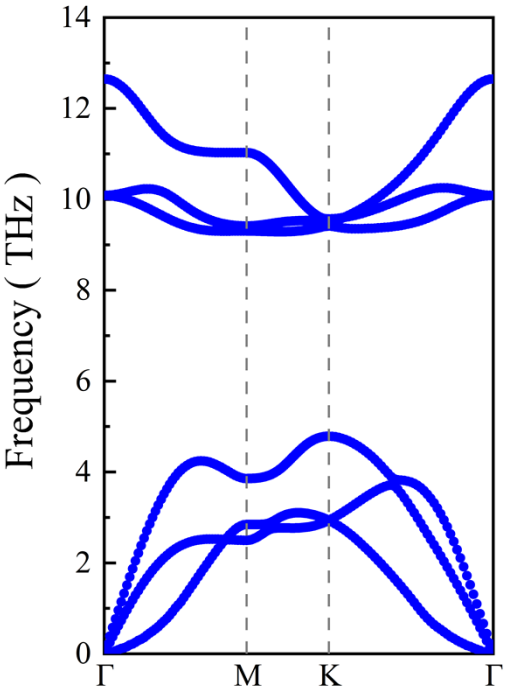

Fig. S2. Phonon spectrum of monolayer *β*-AsP.

3. Molecular dynamics simulations of monolayer *β*-AsP

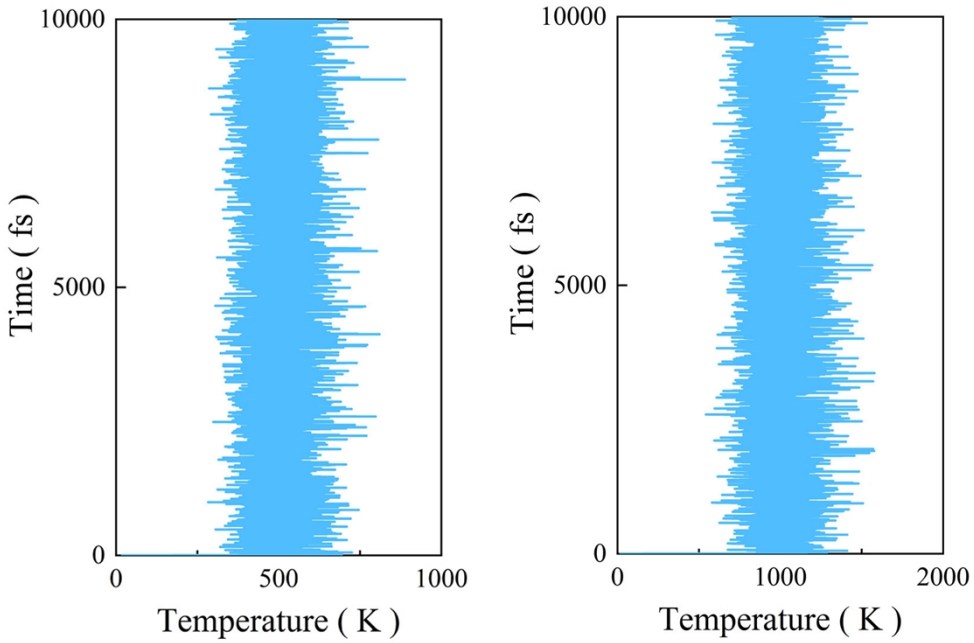

Fig. S3. The free energy variation over time (10.0 ps) of the *β*-AsP monolayer at temperatures of 500 K and 1000 K was obtained through atomic molecular dynamics (AIMD) simulations.

4. Optical properties of *β*-AsP monolayers

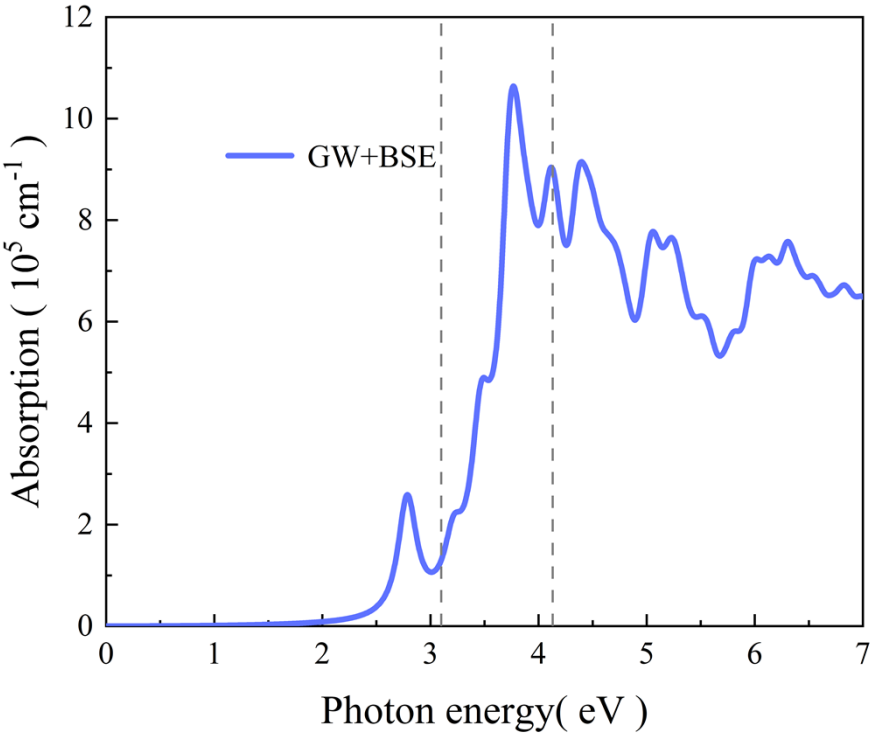

Fig. S4. calculation of light absorption coefficient of *β*-AsP monolayer using GW + BSE method.

5. Electronic structure of monolayer *β*-AsP

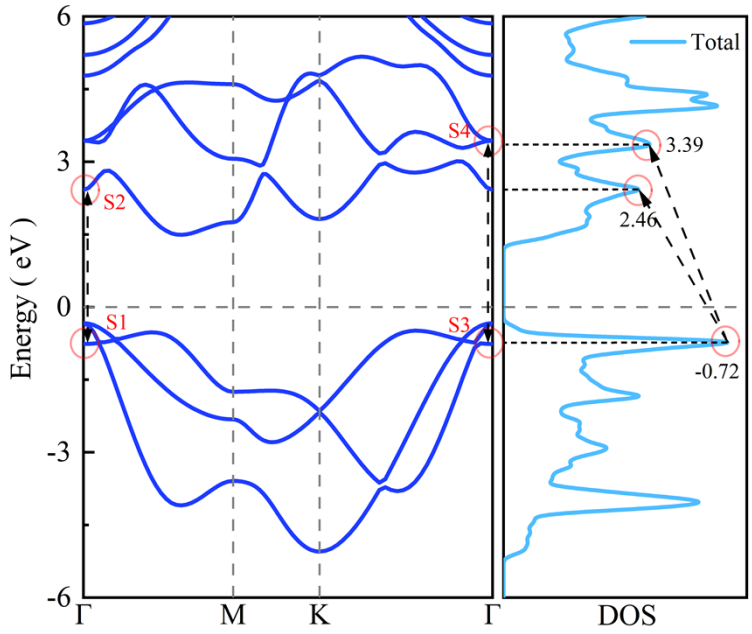

Fig. S5. Band structure and density of states with PBE functional for β-AsP monolayer.