

## Mechanical, electronic and optical properties of novel B<sub>2</sub>P<sub>6</sub> monolayer: ultrahigh carrier mobility and strong optical absorption

Kai Ren,<sup>\*a</sup> Huabing Shu,<sup>b</sup> Wenyi Huo,<sup>a</sup> Zhen Cui,<sup>c</sup> Jin Yu<sup>d</sup> and Yujing Xu<sup>\*e</sup>

<sup>a</sup>*School of Mechanical and Electronic Engineering, Nanjing Forestry University, Nanjing, Jiangsu 210042, China*

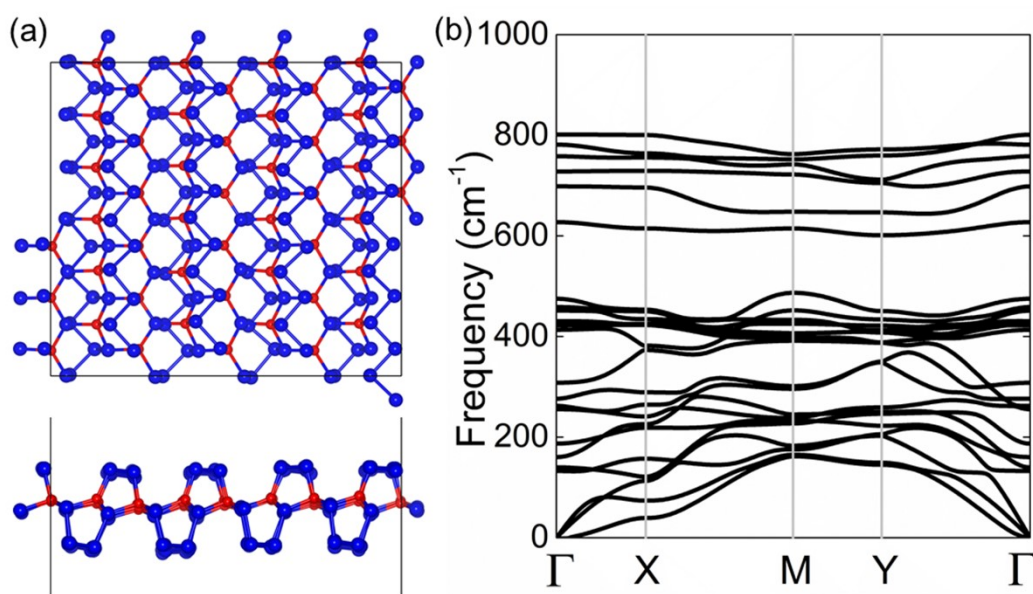
<sup>b</sup>*School of Science, Jiangsu University of Science and Technology, Zhenjiang 212001, China*

<sup>c</sup>*School of Automation and Information Engineering, Xi'an University of Technology, Xi'an, Shaanxi 710048, China*

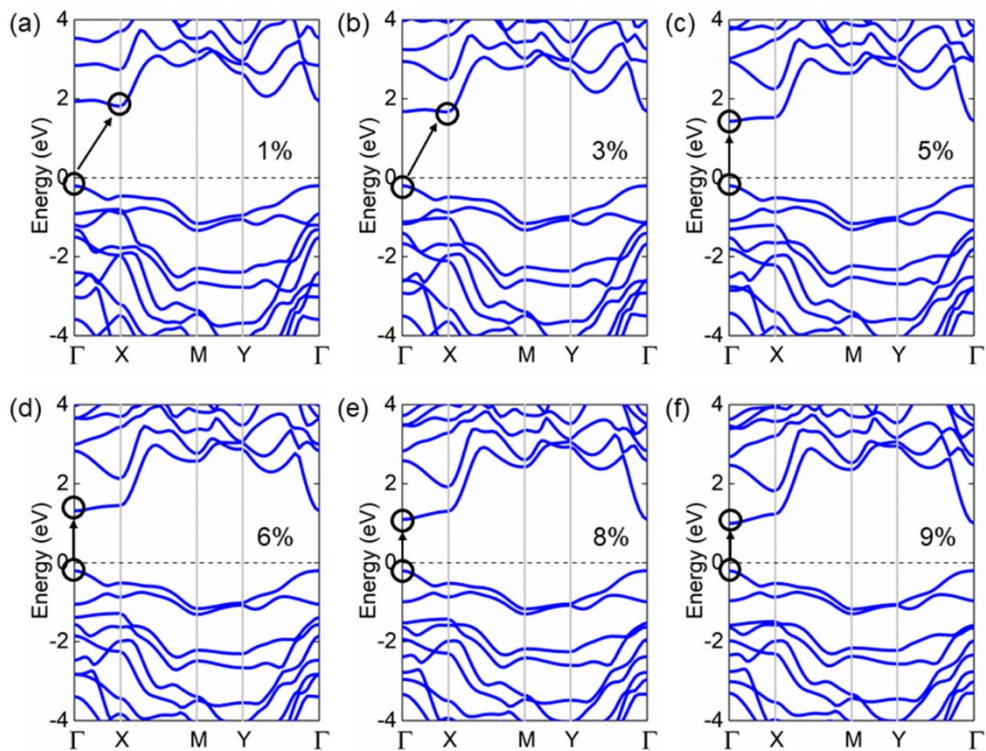
<sup>d</sup>*School of Materials Science and Engineering, Southeast University, Nanjing, Jiangsu 211189, China*

<sup>e</sup>*Independent researcher, China*

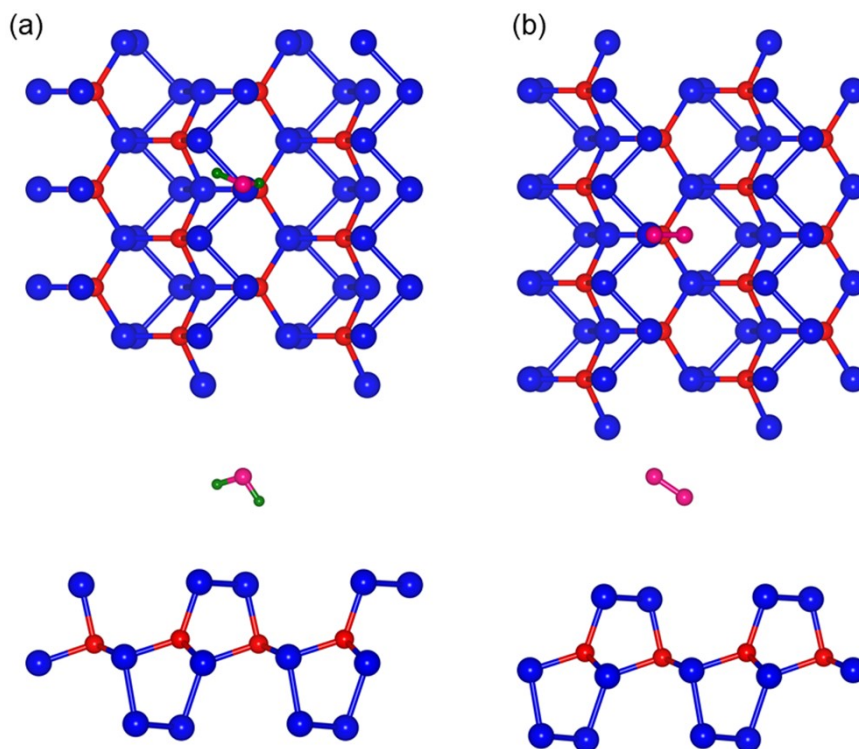
*\*E-mail: kairen@njfu.edu.cn, yujingxusun@gmail.com.*



**Fig. S1** (a) Atomic structure of after 10 ps and (b) the phonon spectrum of the B<sub>2</sub>P<sub>6</sub> monolayer.



**Fig. S2** Band structures of monolayer  $B_2P_6$  under the biaxial tensile strains of (a) 1%, (b) 3%, (c) 5%, (d) 6%, (e) 8% and (f) 9%, respectively, obtained by the HSE06 functional.



**Fig. S3** The optimized structure of the (a)  $H_2O$  and (b)  $O_2$  molecule adsorbed  $B_2P_6$  system.