

Supplementary Information

Magnetic switch and quantization of bandgap in 2D graphene-like CrP₃

Hong-yao Liu^{a, b}, Mi He^c, Huan Yang^{* a}, and Yujun Zheng^{*a}

^aSchool of Physics, Shandong University, Jinan 250100, China

^bSchool of Information and Electronic Engineering, Shandong Technology and
Business University, Yantai 264005, China

^cShenzhen Jingtai Technology Co., Ltd. (XtalPi), Shenzhen 518045, China

*E-mail: h.yang@sdu.edu.cn, yzheng@sdu.edu.cn

List of Supplementary Figures

Fig. S1 The phonon dispersion spectra of the p-CrP₃ and g-CrP₃
monolayers

Fig. S2 The formation energies in the convex hull diagram of the two
types of CrP₃

Fig. S3 The variation of MAE of g-CrP₃ monolayer with U value

Fig. S4 The band structure changes of g-CrP₃ under different strains

Fig. S5 The band structure changes of p-CrP₃ under different strains

Fig. S6 The band structure of g-CrP₃ by HSE06 functional

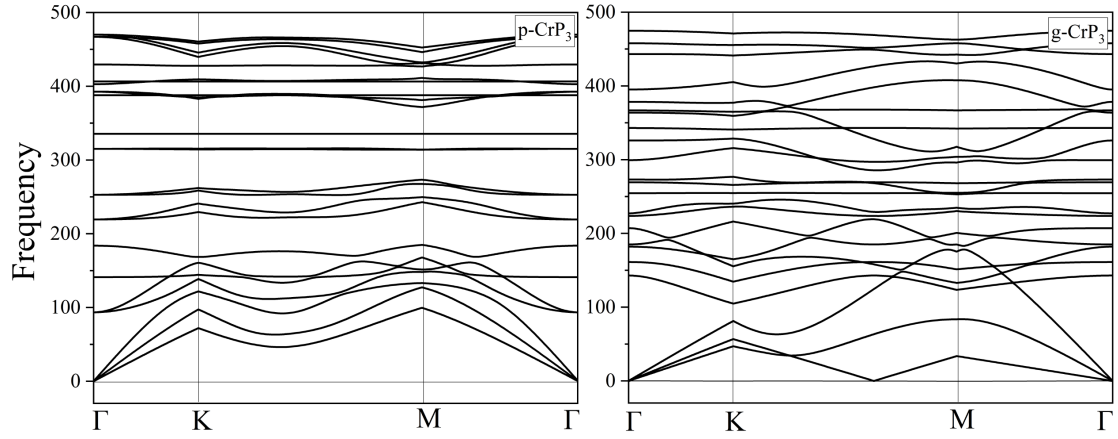


Fig. S1. The phonon dispersion spectra of the p-CrP₃ and g-CrP₃.

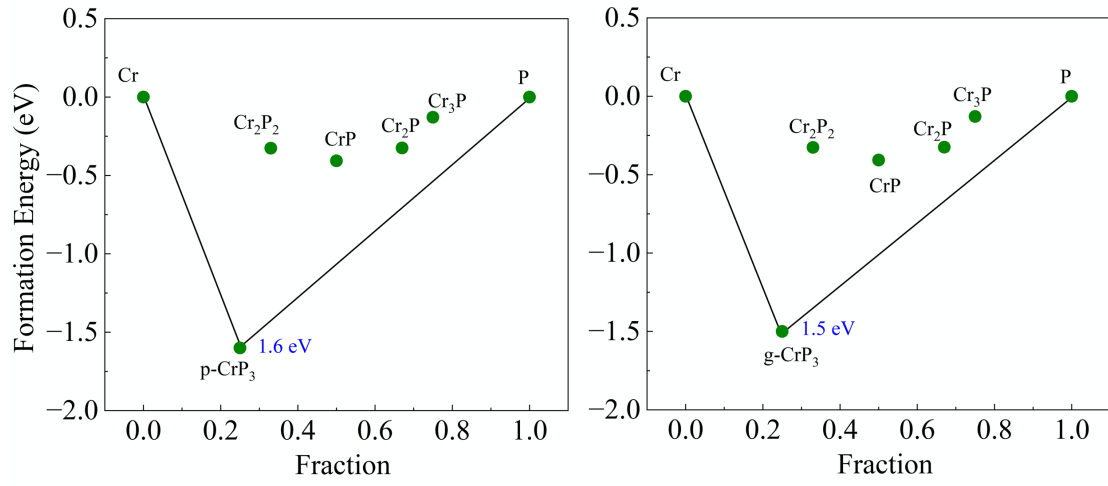


Fig. S2. The formation energies in the convex hull diagram of the two types of CrP₃.

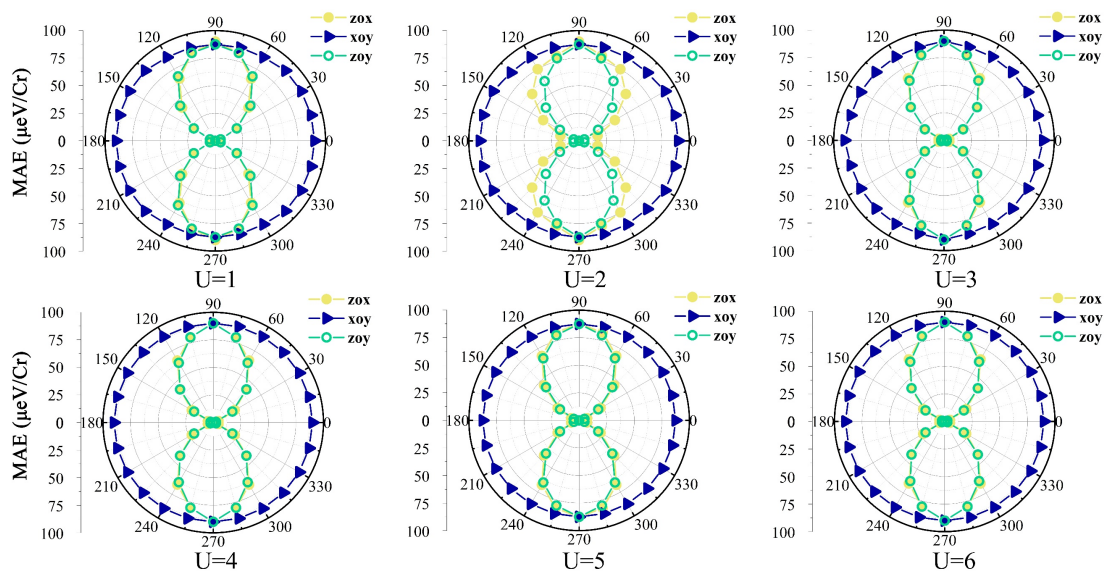


Fig. S3. The variation of MAE of g-CrP₃ monolayer with U value.

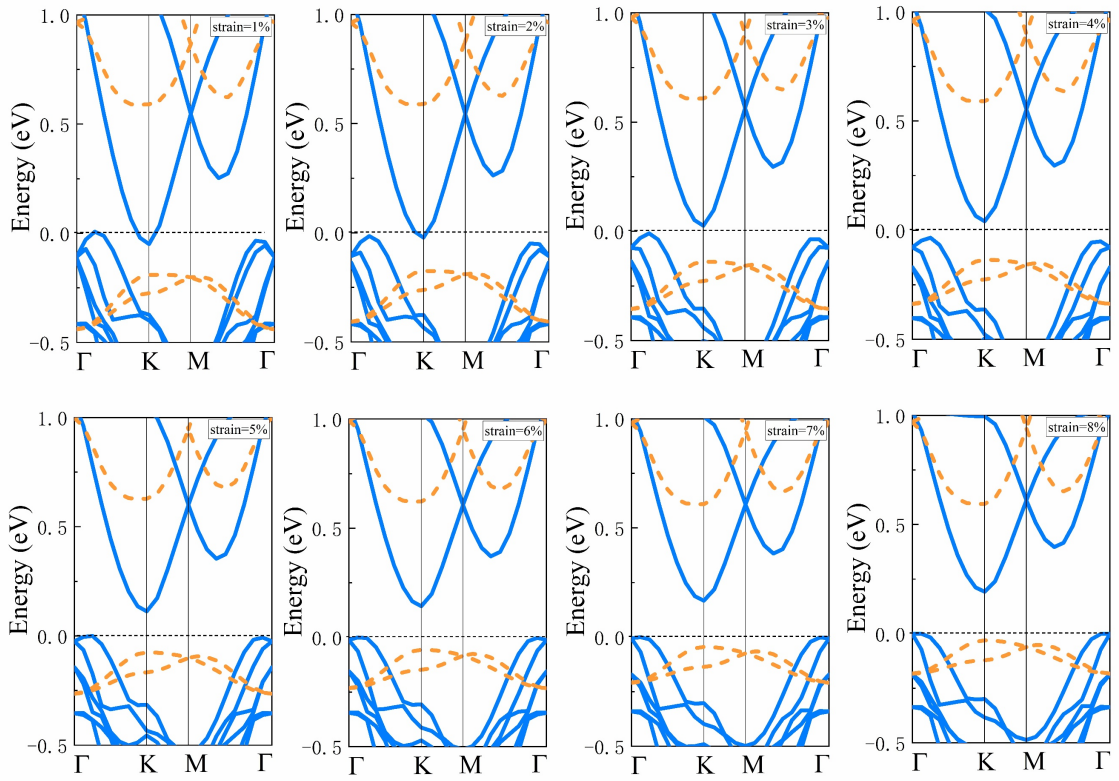


Fig. S4. The band structure changes of g-CrP₃ under different strains, where the blue solid line represents spin up and the orange dashed line represents spin down.

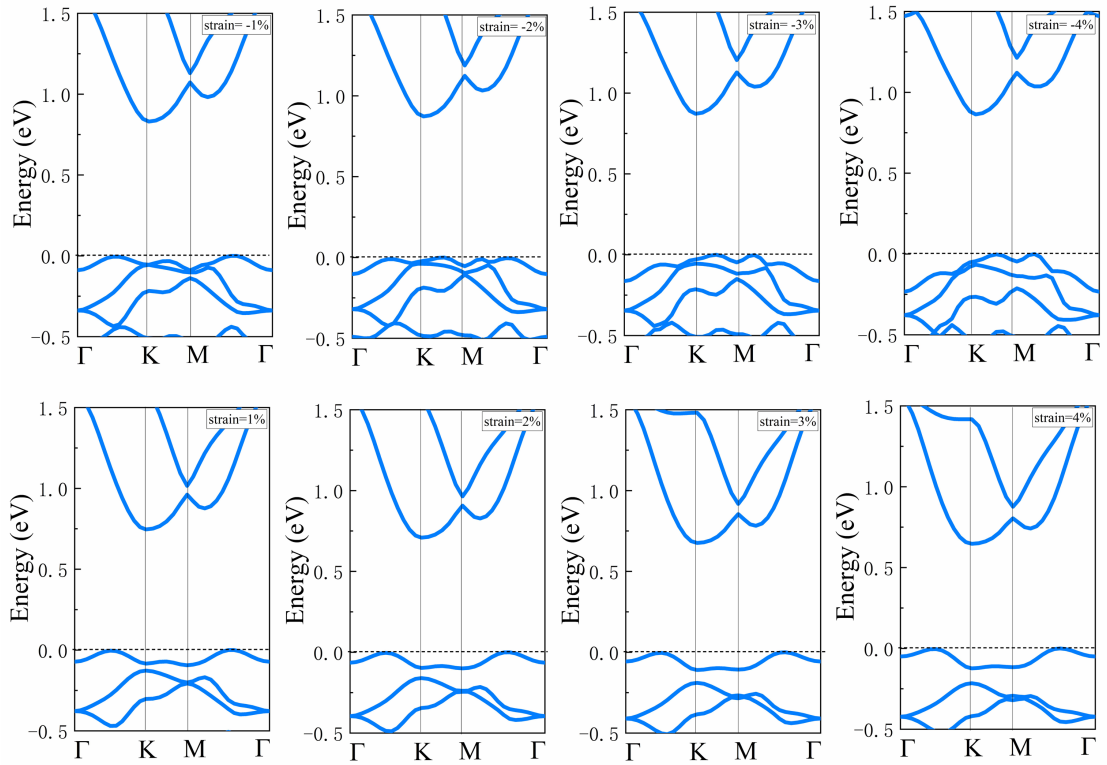


Fig. S5. The band structure changes of p-CrP₃ under different strains.

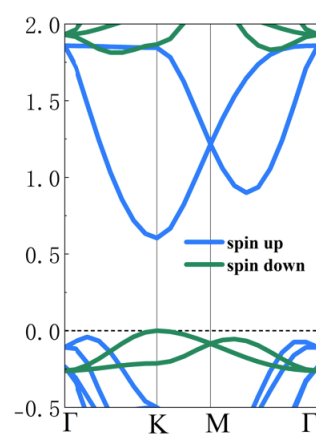


Fig. S6. The band structure of g-CrP3 by HSE06 functional.