

Supplementary Information

Theoretical study of piezoelectric, light absorption properties, and carrier
mobilities of Janus TiPX (X = F, Cl, Br) monolayers

Tong-Tong Yan^a, Guo-Xiang Zhou^{a*}, Xiao-Long Jiang^a, Xu-Chen Qin^a, Jia Li^b

^aSchool of Science, Hebei University of Technology, Tianjin 300401, China

^bCollege of Science, Civil Aviation University of China, Tianjin 300300, China

*Corresponding author. E-mail address: zhouguoxiang@hebut.edu.cn.

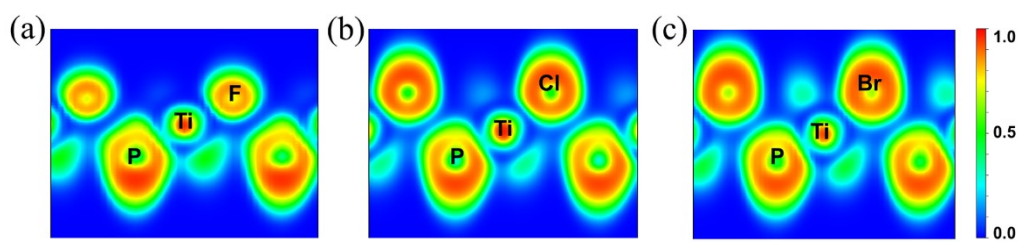


Fig. S1 (a) Calculated electron localization function (ELF) of monolayers (a) TiPF, (b) TiPCL, and (c) TiPBr. ELF = 1.0 stands for perfect localization, ELF = 0.5 corresponds to the free electron gas, and ELF = 0 means the absence of electrons.

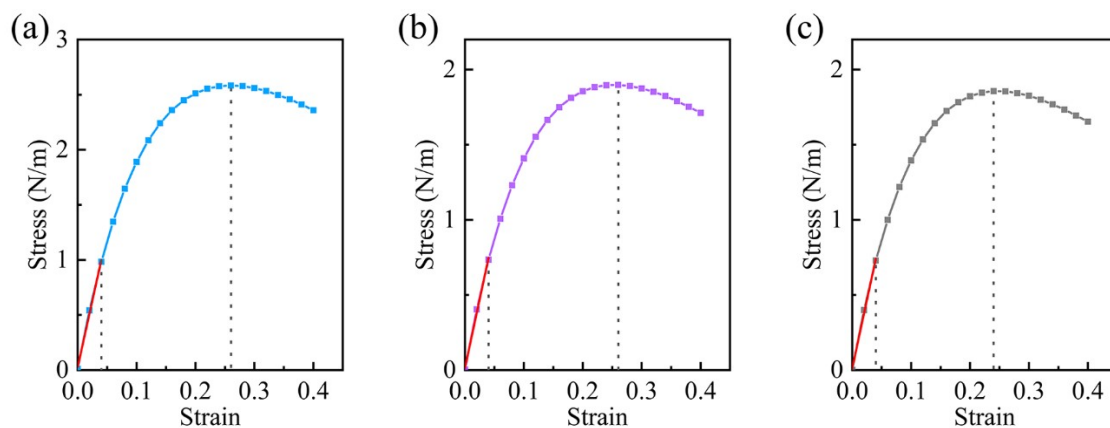


Fig. S2 Stress-strain curves of the monolayers (a) TiPF, (b) TiPCl, and (c) TiPBr. The red line indicates a linear, proportional relationship between stress and strain.

The results show a linear relationship between stress and strain in the range of 4%. The critical strains (monolayer up to fracture) for TiPF, TiPCl, and TiPBr are about 26%, 26%, and 24%, meanwhile, the corresponding calculated tensile stresses are 2.58, 1.90, and 1.86 N/m, respectively.

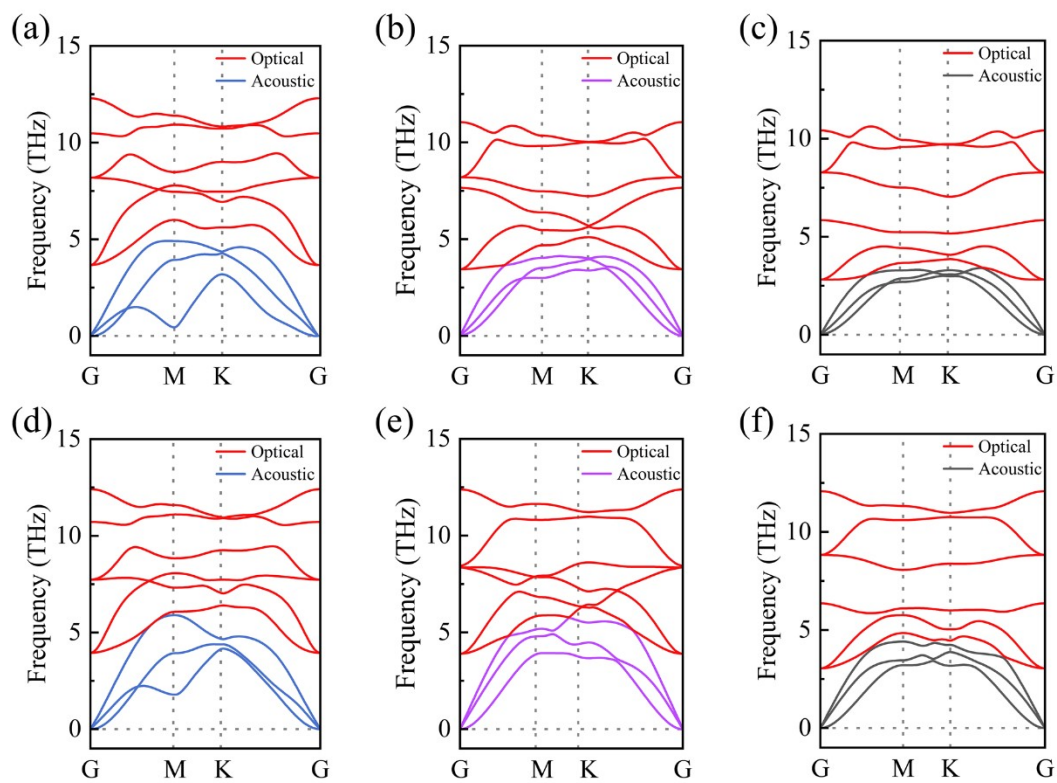


Fig. S3 Phonon spectra of Janus TiX monolayers. 4% biaxial strain for (a)TiPF (b) TiPCl and (c) TiPBr. -4% biaxial strain for (d) TiPF (e) TiPCl (f) TiPBr.

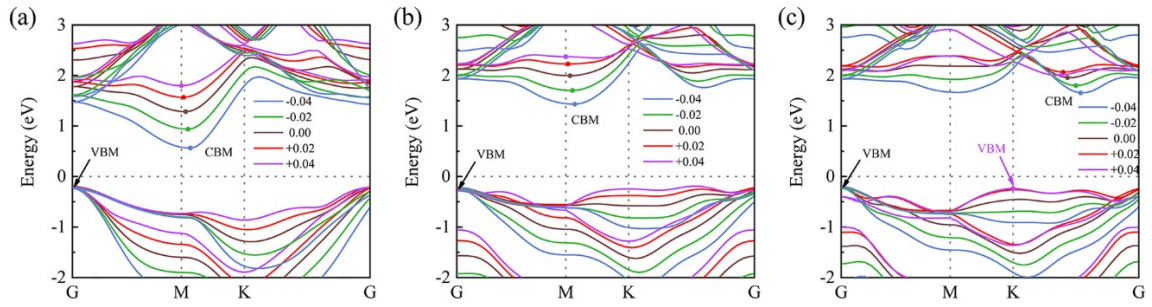


Fig. S4 Electronic band structures of monolayers (a) TiPF, (b) TiPCL, and (c) TiPBr at $\pm 4\%$, $\pm 2\%$, and 0% strain, in which blue, green, brown, red, and purple are applied to represent bands at -4% , -2% , 0% , $+2\%$, and $+4\%$ strain, respectively. The CBM positions of each band are represented by points of the same color as the band, and the VBM positions are indicated by arrows.

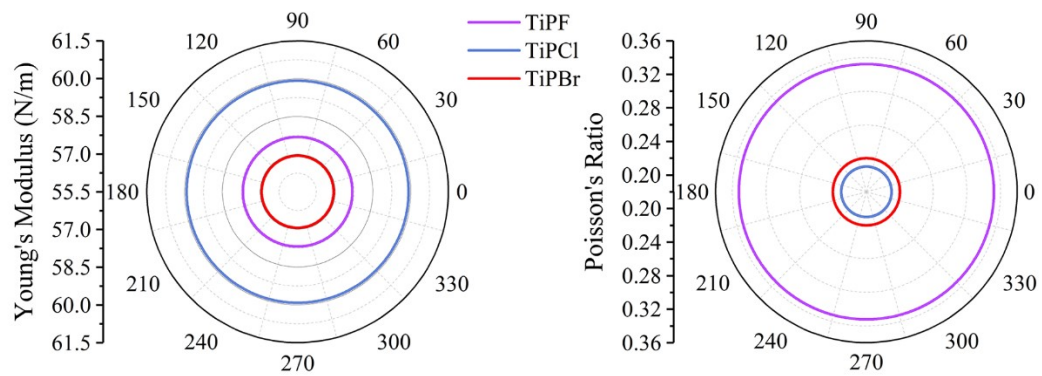


Fig. S5 The variation of Young's modulus and Poisson's ratio in the xy plane of TiPX monolayers.

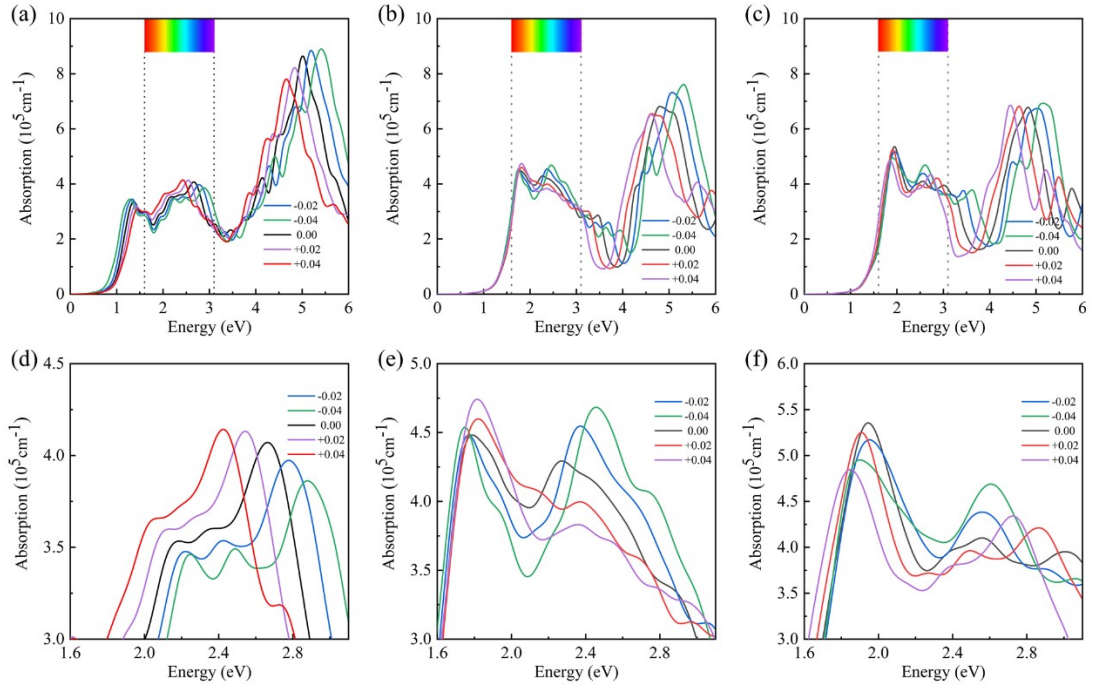


Fig. S6 The light absorption properties of (a) TiPF, (b) TiPCL, and (c) TiPBr at strains ranging from -4% to 4%. Amplified light absorption spectra of (d) TiPF (e) TiPCL and (f) TiPBr in the visible light energy range (1.6~3.1 eV).