Vanishing Schottky Barriers in Blue Phosphorene/MXene Heterojunctions

Hefei Wang[1], Chen Si[1,2], Jian Zhou[1,2], Zhimei Sun[1,2*]

[1]School of Materials Science and Engineering, Beihang University, Beijing 100191, China

[2]Center for Integrated Computational Materials Engineering, International Research Institute for Multidisciplinary Science, Beihang University, Beijing 100191, China

*Correspondence and requests for materials should be addressed to Z. M. Sun: E-mail: zmsun@buaa.edu.cn

1. Calculations for possible magnetism in freestanding MXenes and BlueP/MXene heterojunctions

Table S1. The calculated total magnetic moment for Zr-, Hf- and Nb-based MXenes and BlueP/MXene heterojunctions.

System	Magnetic Moment (μ_B)
Zr_2C	1.20
Zr_3C_2	1.51
Zr_4C_3	1.80
Hf_3C_2	0.94
Hf_4C_3	1.37
BlueP/Zr_3C_2	1.30
BlueP/Zr_4C_3	1.57

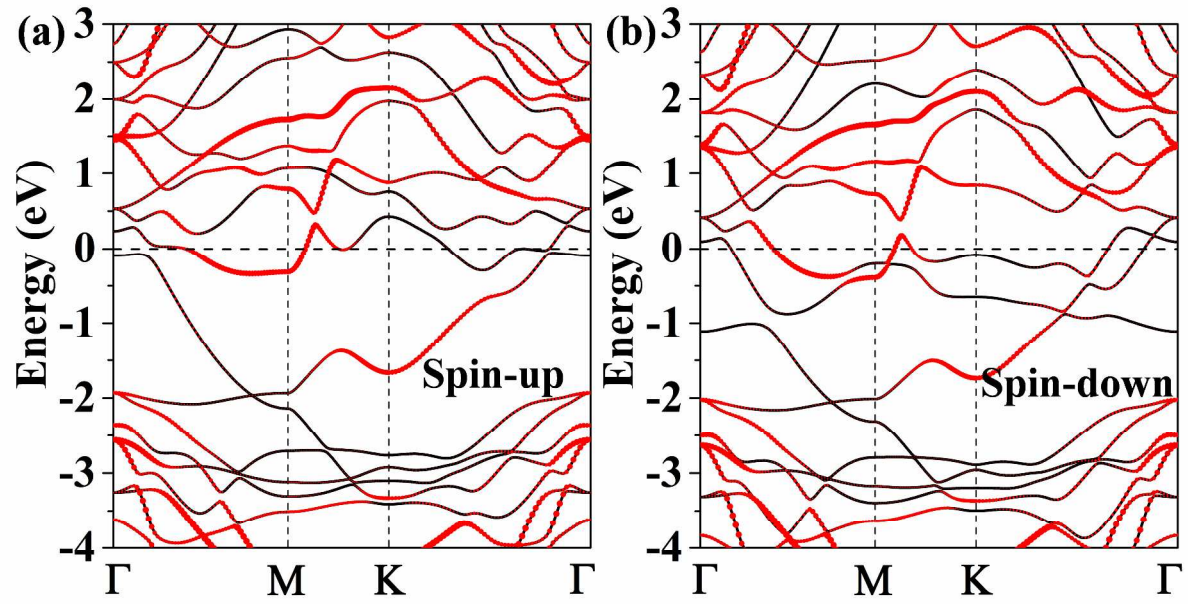

Figure S1. Spin-polarized projected band structures of BlueP/Zr_3C_2 heterojunctions. Two spin channels are marked in the figures. The contribution from BlueP electronic orbitals is represented by red circles in the band structures. The Fermi level is set at zero.

2. Different stacking patterns for BlueP/MXene heterojunctions

We consider six possible stacking patterns for all BlueP/MXene heterojunctions. The various configurations for BlueP/M_2C are shown in Figure S2. The patterns for Heterojunctions composed of BlueP and other MXenes can be obtained in the same way. Among these patterns, the most stable one is chosen to perform the calculation for electronic and interfacial properties.

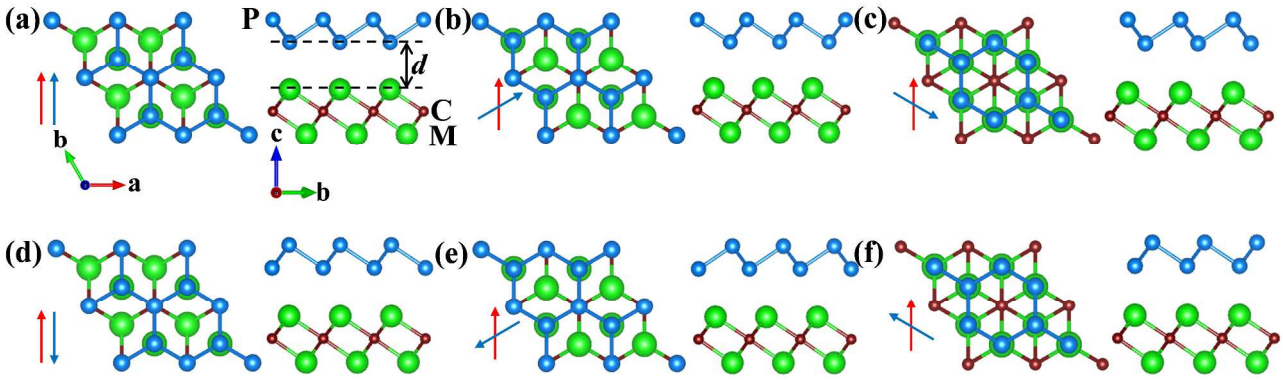

Figure S2. The schematic diagram of the crystal structure of BlueP/M_2C (M = Zr, Hf, Nb) heterojunction with different stacking patterns. The rotation angles of BlueP with respect to M_2C are (a) 0°, (b) 60°, (c) 120°, (d) 180°, (e) 240° and (f) 300°, respectively.

3. Electronic structure calculations for BlueP/MXene heterojunctions with HSE06 hybrid functional

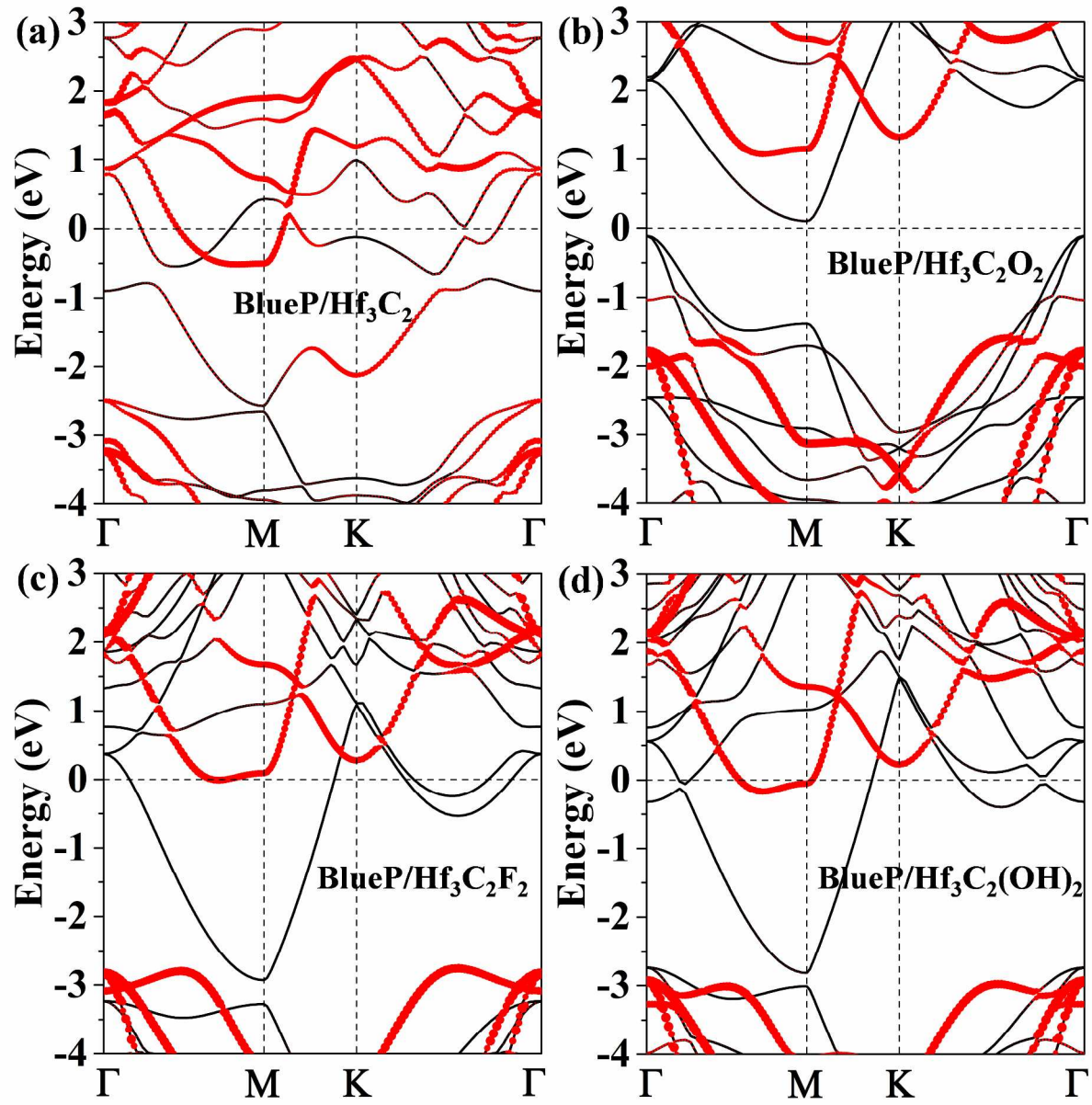

Figure S3. Projected band structures of (a) BlueP/Hf_3C_2, (b) BlueP/$Hf_3C_2O_2$, (c) BlueP/$Hf_3C_2F_2$ and (d) BlueP/$Hf_3C_2(OH)_2$ heterojunctions based on the HSE06 functional. The contribution from BlueP electronic orbitals is represented by red circles in the band structures. The Fermi level is set at zero.

4. The examination of the effect of small strains on the electronic structures for BlueP/MXene heterojunctions.

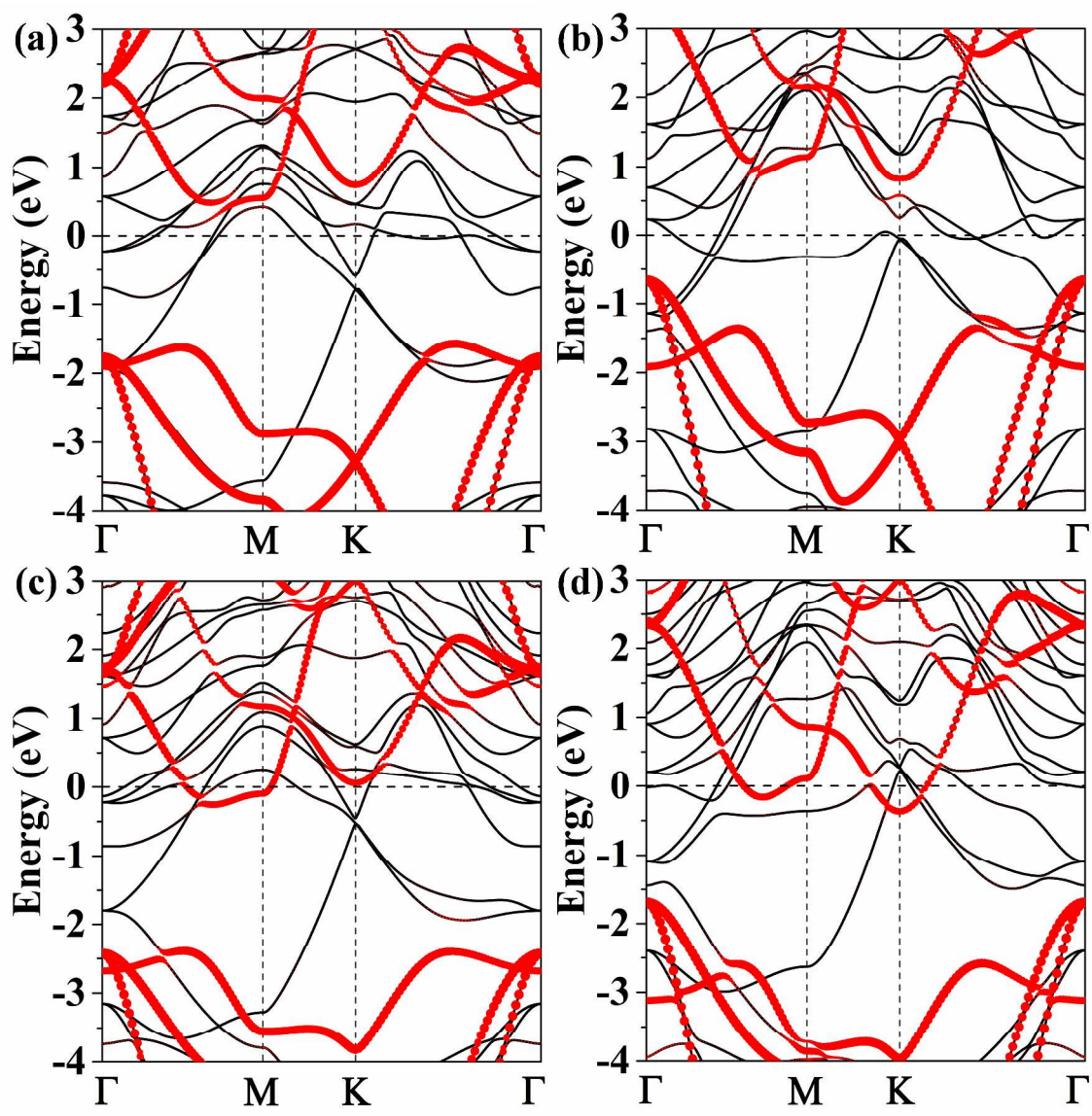

Figure S4. Projected band structures of (a), (b) BlueP/$Nb_3C_2F_2$ and (c), (d) BlueP/$Nb_3C_2(OH)_2$ where (a) and (c) are calculated by fixing the lattice constant of BlueP, while (b) and (d) are obtained by fixing the lattice constants of corresponding MXenes. Compared with other heterojunctions, these MXenes have the largest lattice mismatches with BlueP in the two systems. The contribution from BlueP is represented by red circles in the band structures. The Fermi level is set at zero.

5. The examination of the spin-orbit coupling (SOC) effect on the electronic structures for BlueP/MXene heterojunctions.

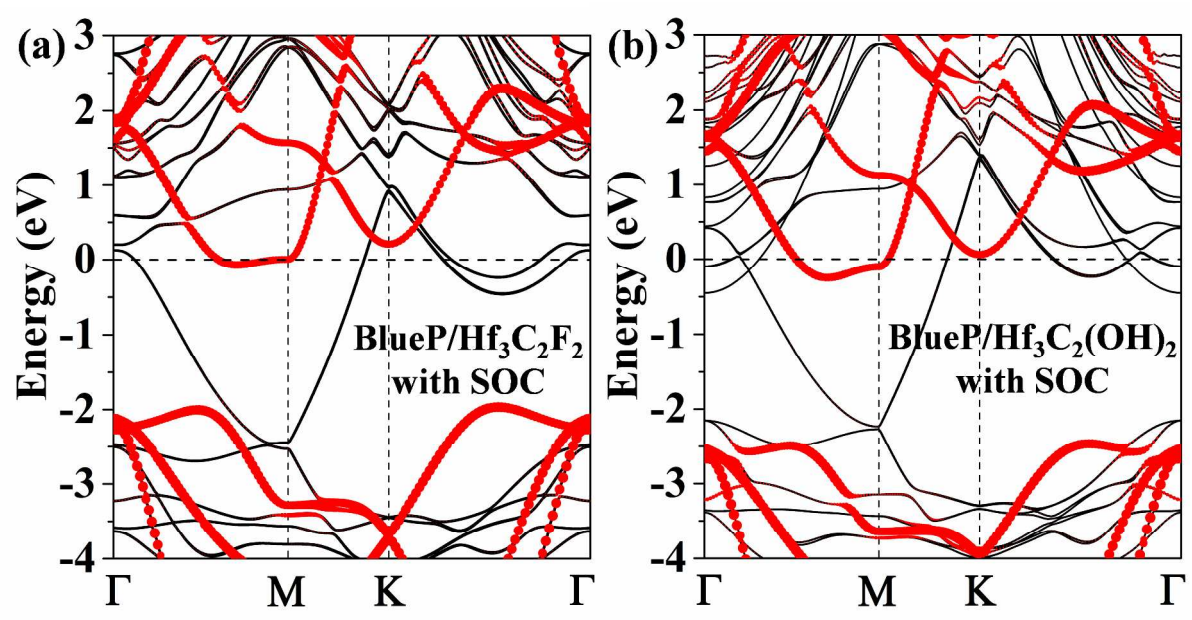

Figure S5. Projected band structures of (a) BlueP/$Hf_3C_2F_2$ and (b) BlueP/$Hf_3C_2(OH)_2$ heterojunctions with the spin-orbit coupling (SOC). The contribution from BlueP electronic orbitals is represented by red circles in the band structures. The Fermi level is set at zero.