

Supporting Information for:

**Stacking sequences of black phosphorous allotropes and corresponding few-
layer phosphorenes**

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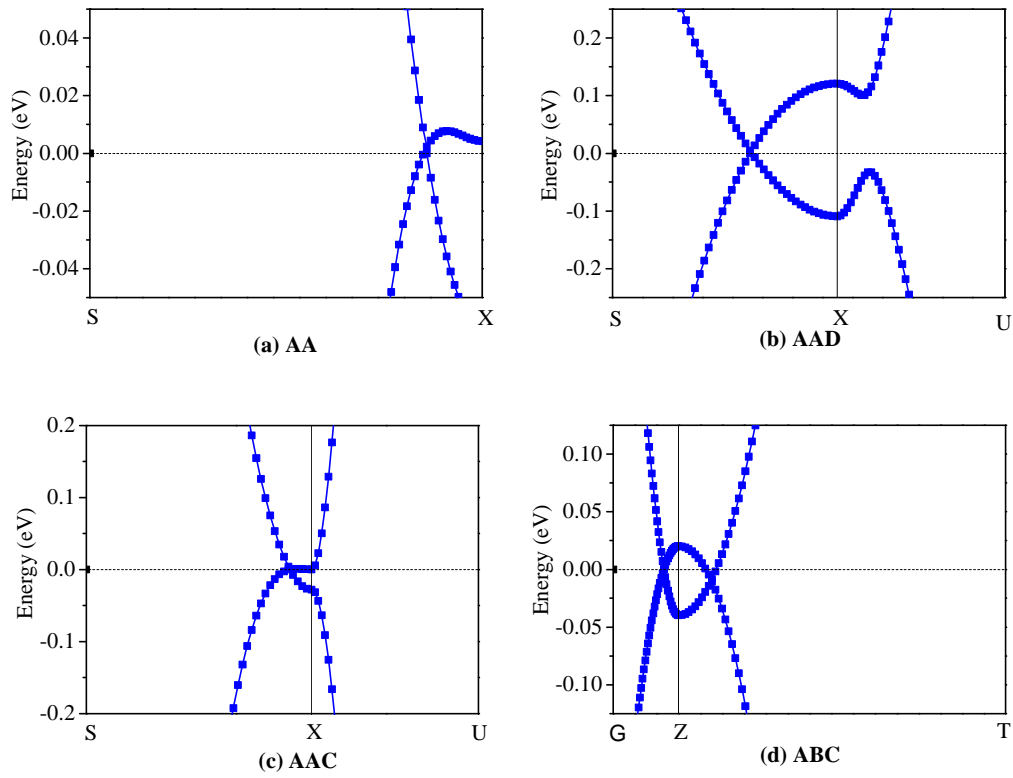


Figure S1. Enlarged band structures of AA, AAC, AAD, and ABC BP allotropes with denser points around the Fermi level. The small band gap of 0.002 eV in the AA structure will reach zero if much denser points are added between the S and X points and Dirac cones will be formed. Therefore, the band structure of AA allotrope shows three-dimensional Dirac semimetal features. The same features can also be observed in the AAC and AAD structures. The ABC structure shows metallic feature because of the bands crossing the Fermi level.

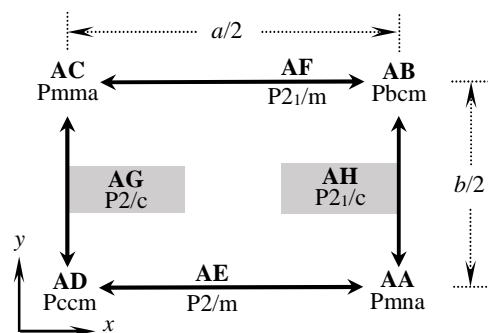


Figure S2. Schematic structural relationships of the bilayer phosphorene structures displayed based on their crystal symmetries. The black solid arrows indicate the possible phase transition path by interlayer slipping. The AG and AH structures marked with grey color are not stable at zero pressure and will transform to other structures after relaxation. The empty spaces could be filled by the various structures with relatively low symmetries, which are not annotated here.

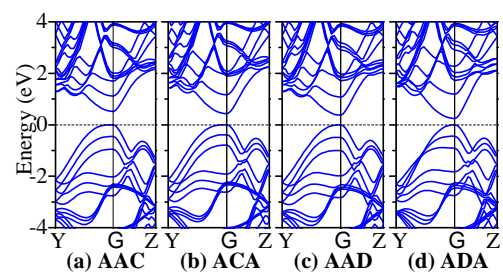


Figure S3. The calculated band structures of the few-layer structures of AAC, ACA, AAD, and ADA.

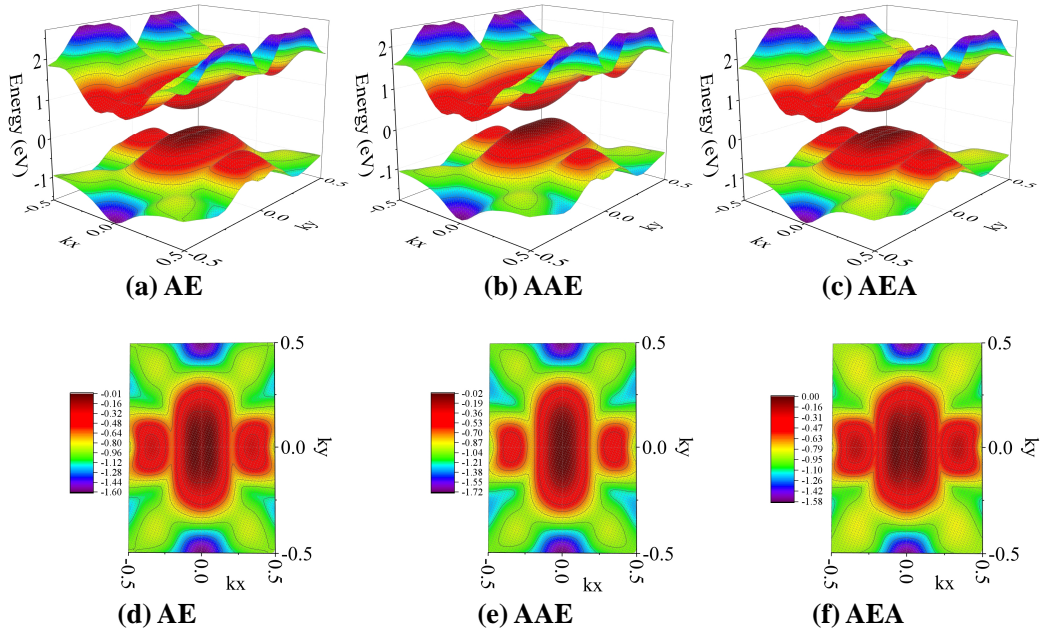


Figure S4. (a-c) Three-dimensional band structures and (d-f) the corresponding projection of the valance band of the few-layer phosphorene structures of AE, AAE, and AEA, respectively. The CBM are all located at the Γ point for these three structures, while the VBM are located at the points marked with the dark red color. The VBM of the AE and AEA structures are clearly located along the Γ -Z direction, while the VBM of the AAE structure is slightly obscure. The band structure calculated using HSE06 shows that the VBM of the AAE structure is quite close to the Γ point along the Γ -Y direction.