Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary information for

Boron-Pnictogen Monolayers with Negative Poisson's ratio and Excellent Band Edge Positions for Photocatalytic Water Splitting.

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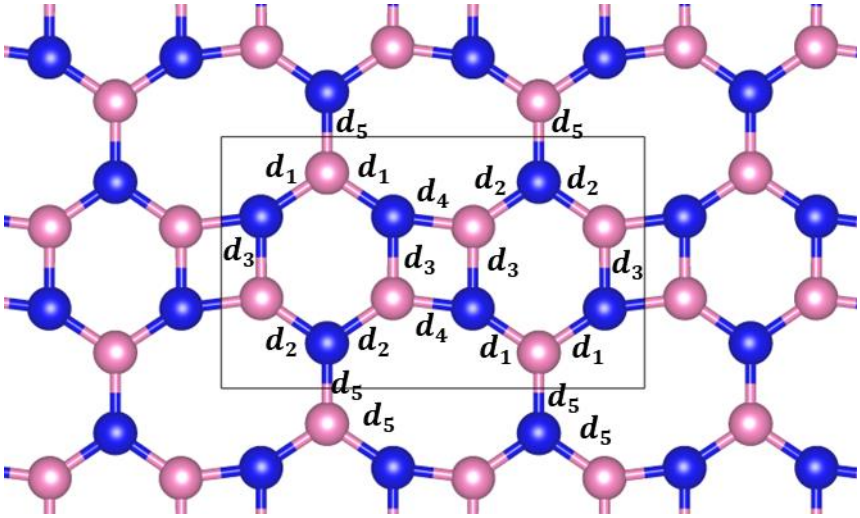

Figure S1. Atomic bond lengths of bp-BX nanosheets. The pink spheres represent the boron and the blue spheres represent the pnictogen (X = N, P, As and Sb) atom.

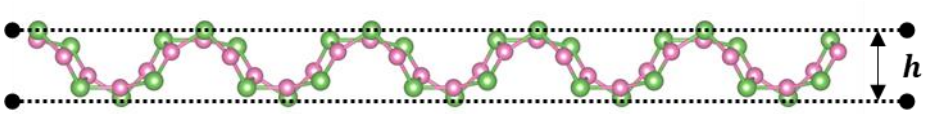

Figure S2. Out-of-plane buckling height (h) of bp-BX nanosheets, (X = P, As, Sb).

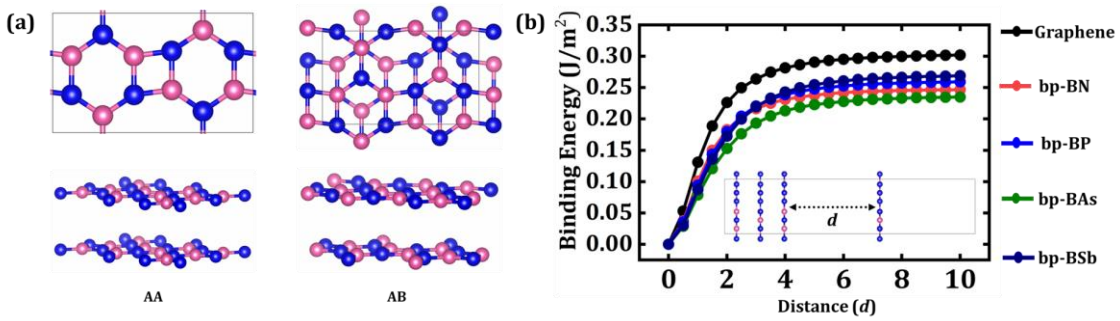

Figure S3. (a) AA and AB-type stacking of bp-BX (X = N, P, As, Sb) 3D phases and (b) computed interlayer binding energy of bp-BX (X = N, P, As, Sb) nanosheets and graphene.

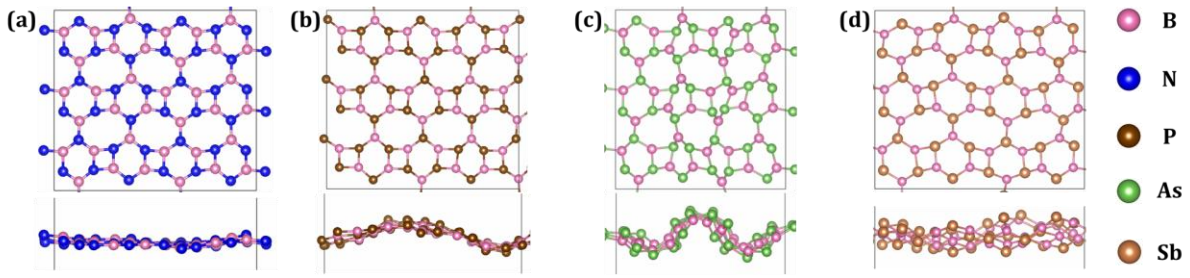

Figure S4. Snapshots of simulated structures of the bp-BX monolayers at the end of 10 picoseconds AIMD simulation.

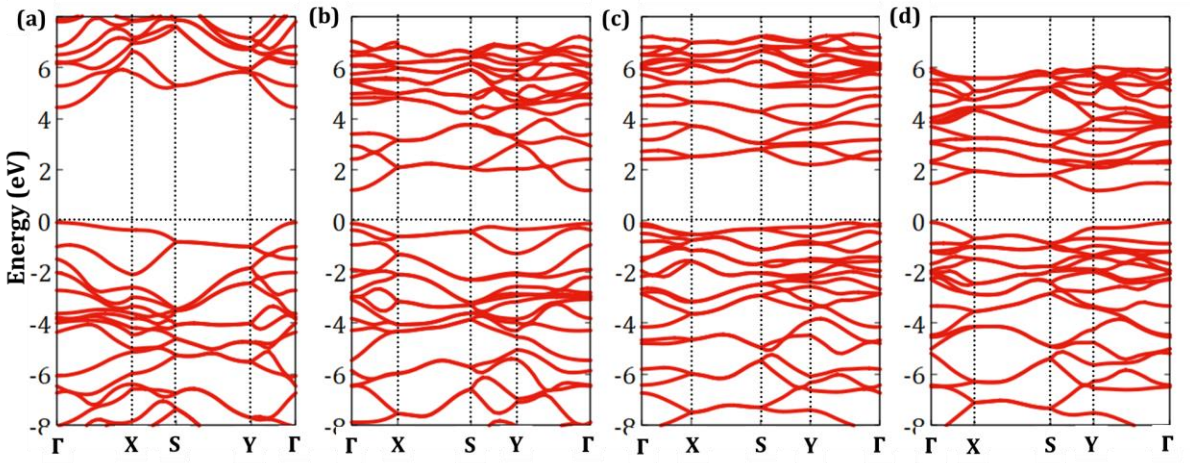

Figure S5. Calculated electronic band structures of bp-BX (X = N, P, As, Sb) nanosheets calculated at HSE06 level of theory. (a) bp-BN, (b) bp-BP, (c) bp-BAs and (d) bp-BSb. The Fermi level is set to zero eV in all cases.

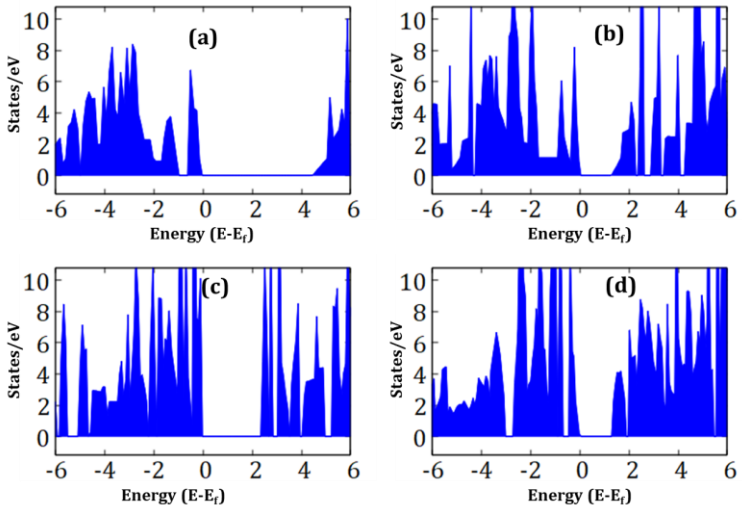

Figure S6. Calculated electronic density of states of bp-BX (X = N, P, As, Sb) nanosheets calculated at HSE06 level of theory. (a) bp-BN, (b) bp-BP, (c) bp-BAs and (d) bp-BSb.

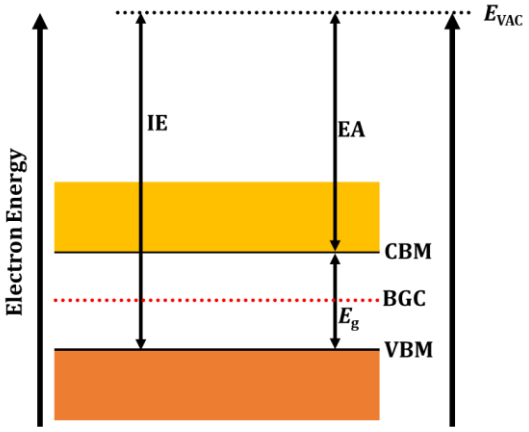

Figure S7. Electronic energy diagram of a semiconductor with energy gap E_g, band edges (CBM and VBM), bandgap centre (BGC), vacuum level (E_{VAC}), ionization energy (IE) and electron affinity (EA).

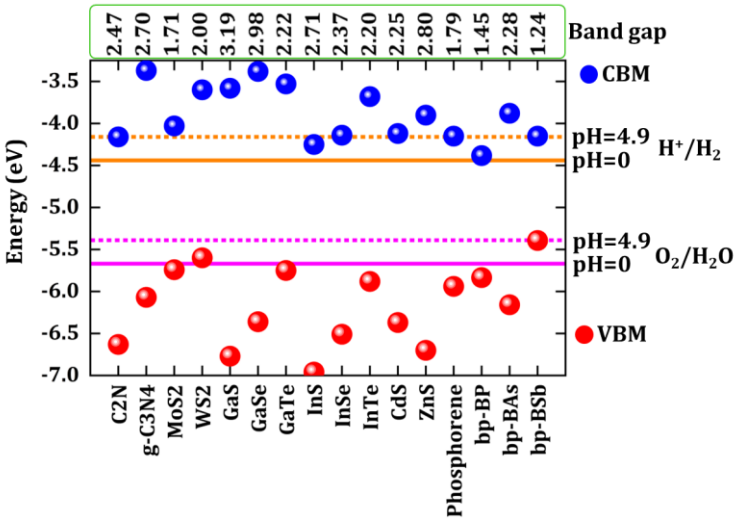

Figure S8. Absolute positions of VBM, CBM, energy gap of different 2D photocatalysts for hydrogen production from water.