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Photocatalysis screening for group III-V vdW heterostructures constructed by MX (M=Ga, In and X=P, As) monolayers

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To harvest solar energy for water splitting and produce pollution-free hydrogen and oxygen, high-performance photocatalysts are essential. Here, by combining different two-dimensional (2D) group III-V MX (M = Ga, In and X = P, As) monolayers, we designed 144 van der Waals (vdW) heterostructures to identify efficient photoelectrochemical materials. Using first-principles calculations, we investigated the stabilities, electronic properties, and optical properties of these heterostructures. After a careful screening process, we elected GaP/InP in a BB-II stacking configuration as the most promising candidate. This specific GaP/InP configuration has a type-II band alignment with a gap value of 1.83 eV. The conduction band minimum (CBM) is located at -4.276 eV, and the valence band maximum (VBM) is located at -6.217 eV, fully satisfying the requirements of the catalytic reaction under pH=0. Additionally, light absorption has been improved through the construction of the vdW heterostructure. These results could help in understanding the properties of the III-V heterostructures and guide the experimental synthesis of these materials for photocatalysis applications.

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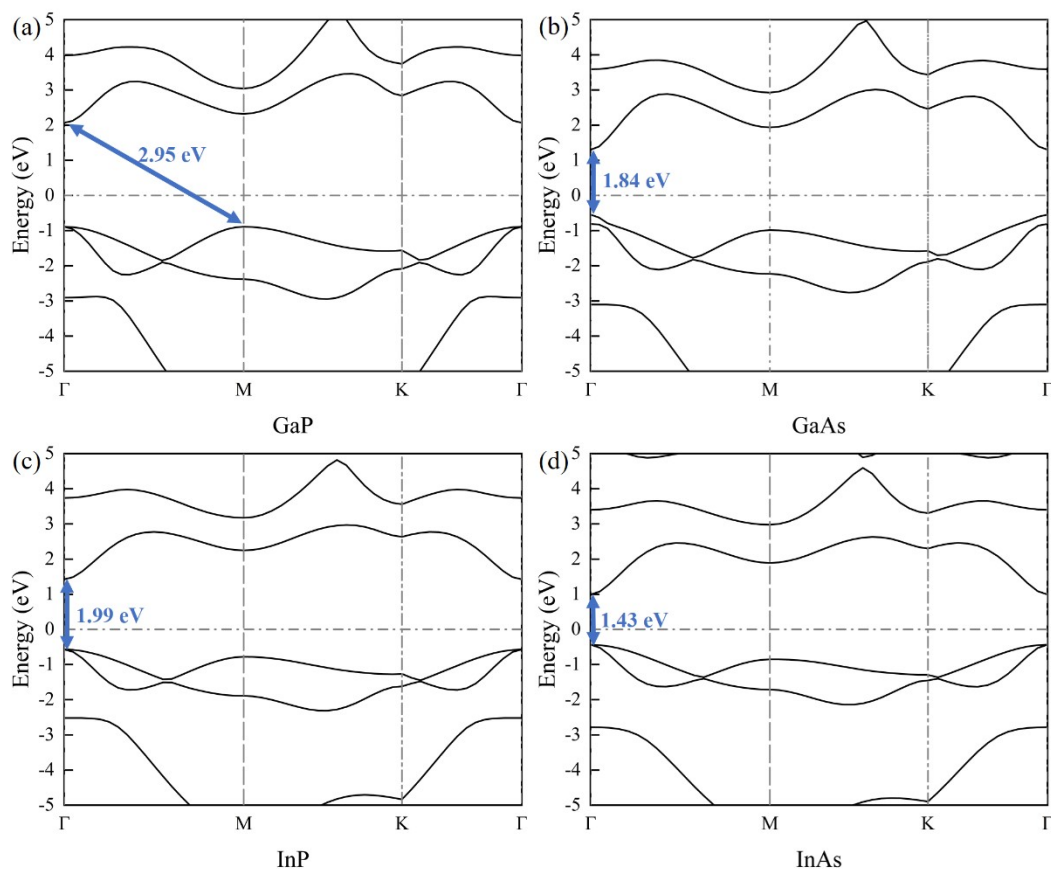† jiabaonan@163.com (B.N. Jia), photon.bupt@gmail.com (P.F. Lu).

Figure S1 The HSE06 band structures of (a) GaP, (b) GaAs, (c) InP, and (d) InAs
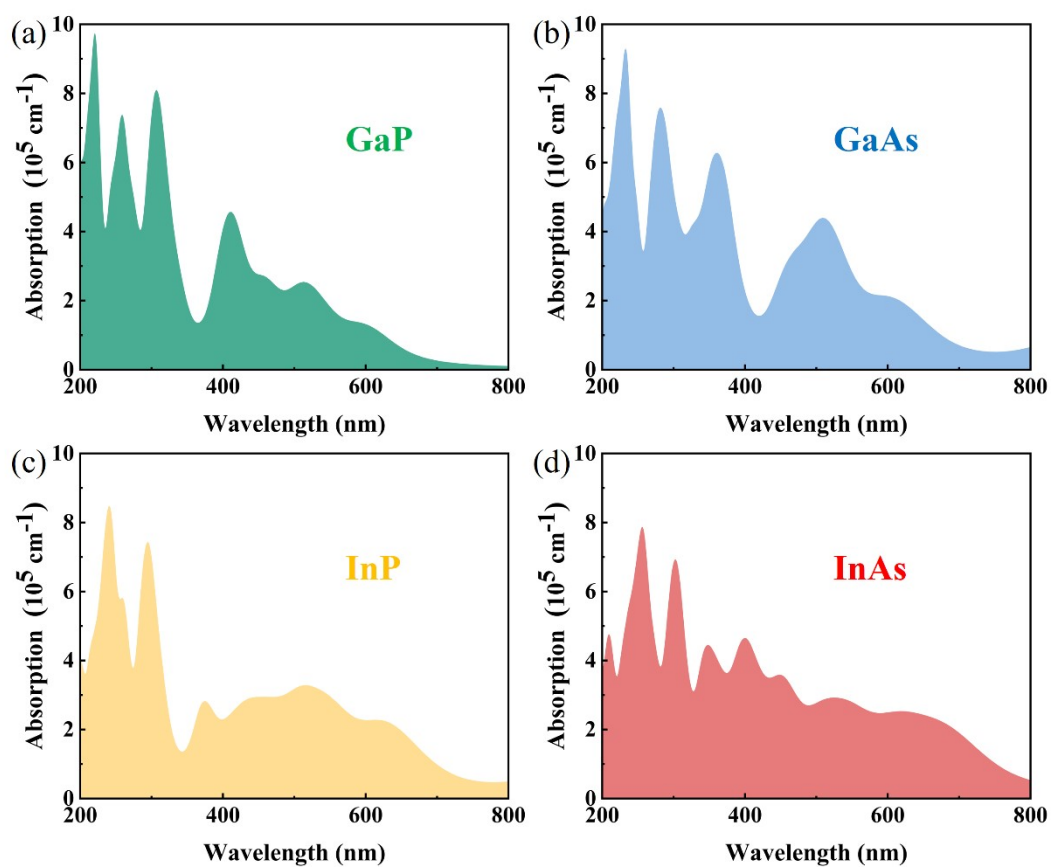
monolayer.

Figure S2 The absorption coefficient α of (a) GaP, (b) GaAs, (c) InP, and (d) InAs monolayer.

Table S1 The lattice constant difference between the top and the bottom layer Δa (Å), the ratio $\Delta a/a_{\text{bottom}}$ (%) and $\Delta a/a_{\text{top}}$ (%).

System	Δa (Å)	$\Delta a/a_{\text{bottom}}$ (%)	$\Delta a/a_{\text{top}}$ (%)
GaP/GaAs	0.1415	3.609	3.483
GaP/InP	0.3258	8.310	7.672
GaP/InAs	0.4558	11.626	10.415
GaAs/InP	0.1843	4.537	4.340
GaAs/InAs	0.3142	7.735	7.180
InP/InAs	0.1299	3.059	2.968

(a) (b) (c)

GaP/GaAs AA-IV GaP/GaAs BB-I GaP/GaAs BB-V

(d) (e)

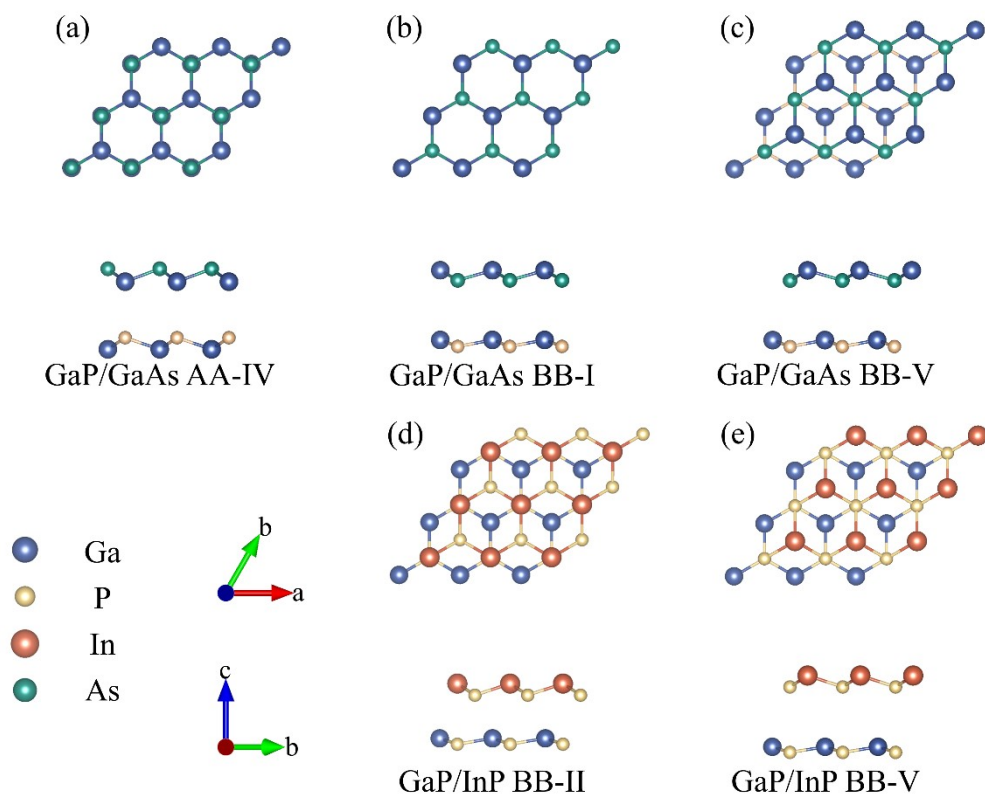- Ga
- P
- In
- As

GaP/InP BB-II GaP/InP BB-V

Figure S3 The side and top views of the five selected configurations: (a) GaP/GaAs (stacking AA-IV), (b) GaP/GaAs (stacking BB-I), (c) GaP/GaAs (stacking BB-V), (d) GaP/InP (stacking BB-II), and (e) GaP/InP (stacking BB-V).