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


# Supporting Information

# A promising photocatalyst of type-II β-AsP/g-$C_6N_6$ van der Waals heterostructure for water splitting: A first-principles study

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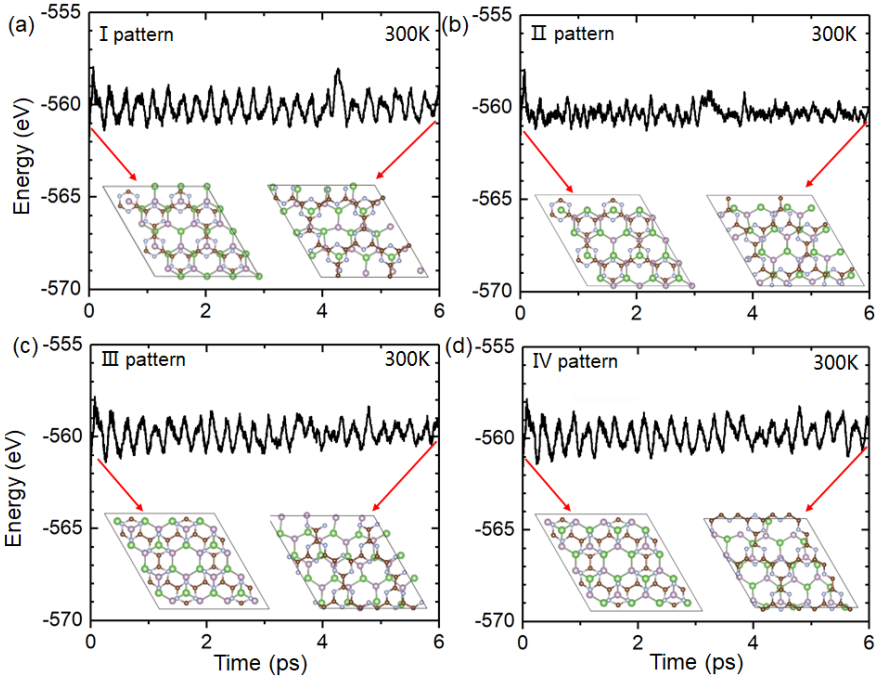


Fig. S1 Variations of energy for β-AsP/g-$C_6N_6$ heterostructure during AIMD simulation lasting for 6 ps at 300 K. The insets represent the top views of initial and final structures in AIMD simulation, respectively.

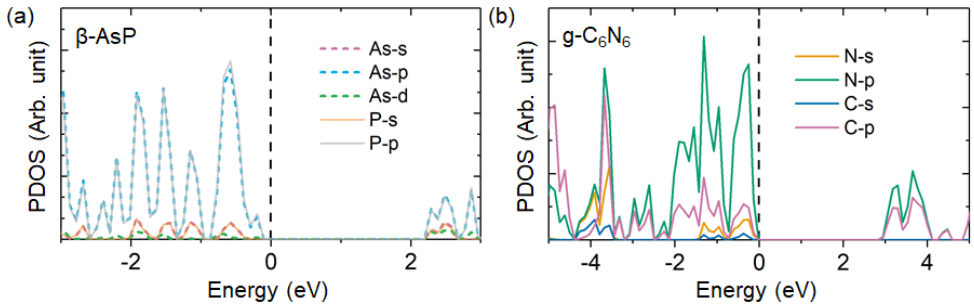


Fig. S2 The density of states of (a) β-AsP and (b) g-$C_6N_6$ monolayers. The Fermi levels are set to 0, represented by the horizontal dotted black lines.

We calculated the band structures of β-AsP and g-$C_6N_6$ monolayer by PBE for comparison, shown in Fig. 1(c-d). β-AsP (g-$C_6N_6$) is an indirect (a direct) semiconductor and their band gaps are 1.89 eV and 2.52 eV, respectively. The gaps are consistent with previous results: 1.84 eV [1] for β-AsP at the PBE level.

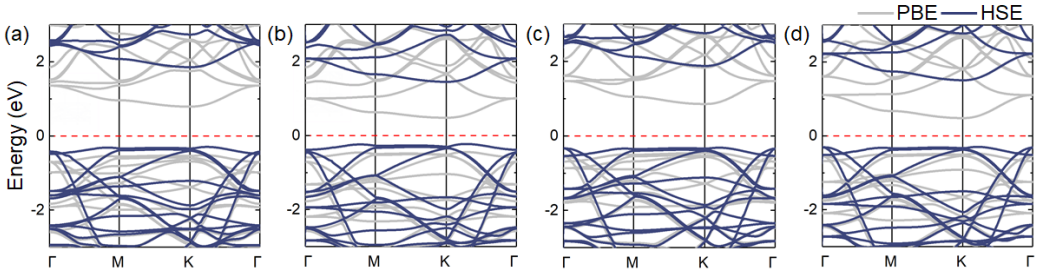


Fig. S3 The band structure of β-AsP/g-$C_6N_6$ heterostructures in (a) I pattern, (b) II pattern, (c) III pattern, and (d) IV pattern by PBE (gray lines) and HSE06 functional (dark blue lines).

The results show that the energy bands calculated by PBE and HSE06 functional are consistent, only the upward shifts of conduction bands and the downward shifts of valence bands. The band gaps by PBE are listed in Table 1.

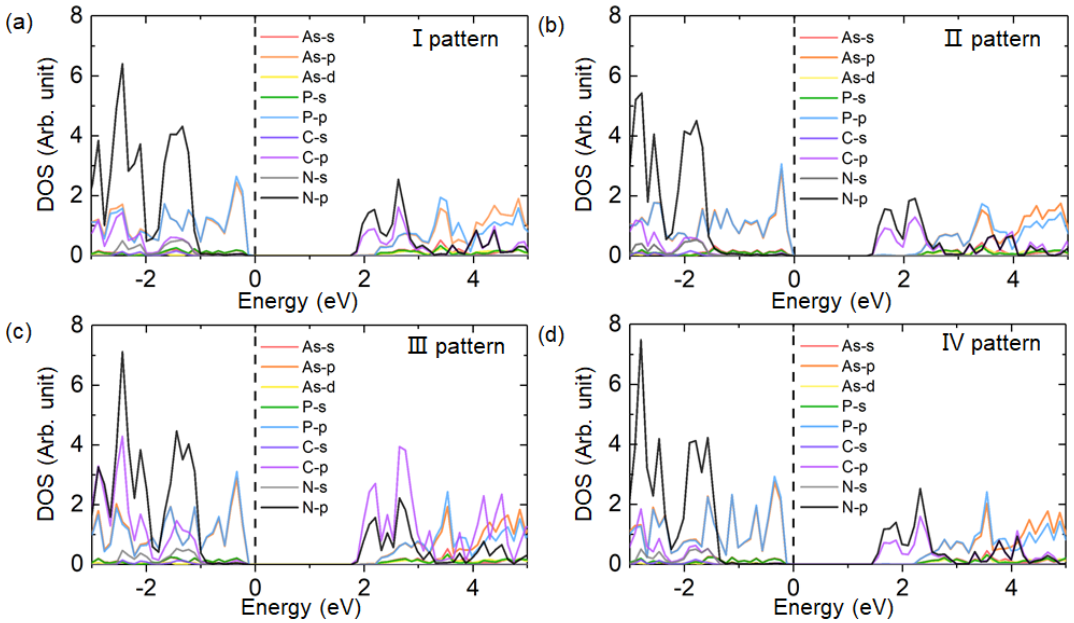


Fig. S4 The density of states of β-AsP/g-$C_6N_6$ heterostructures in (a) I pattern, (b) II pattern, (c) III pattern, and (d) IV pattern. The Fermi levels are set to 0, represented by the horizontal dotted black lines.

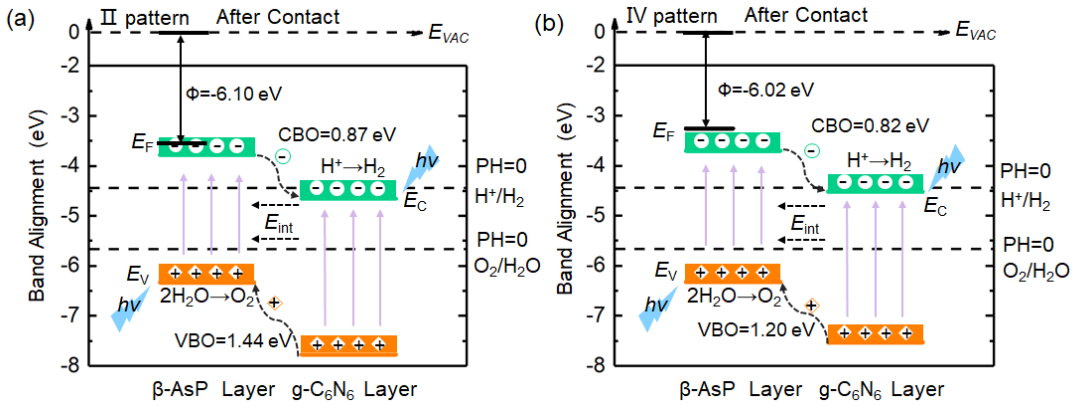


Fig. S5 The schematic diagram of photocatalysis of β-AsP/g-$C_6N_6$ heterostructure in (a) II and (b) IV patterns. The $E_{vac}$ is set to zero.

## References

1. X. Cai, Y. Chen, B. Sun, J. Chen, H. Wang, Y. Ni, L. Tao, H. Wang, S. Zhu, X. Li, *Nanoscale*, 2019, **11**, 8260-8269.