

Janus AsP monolayer: A promising 2D platform for NO and NO₂ gas sensing

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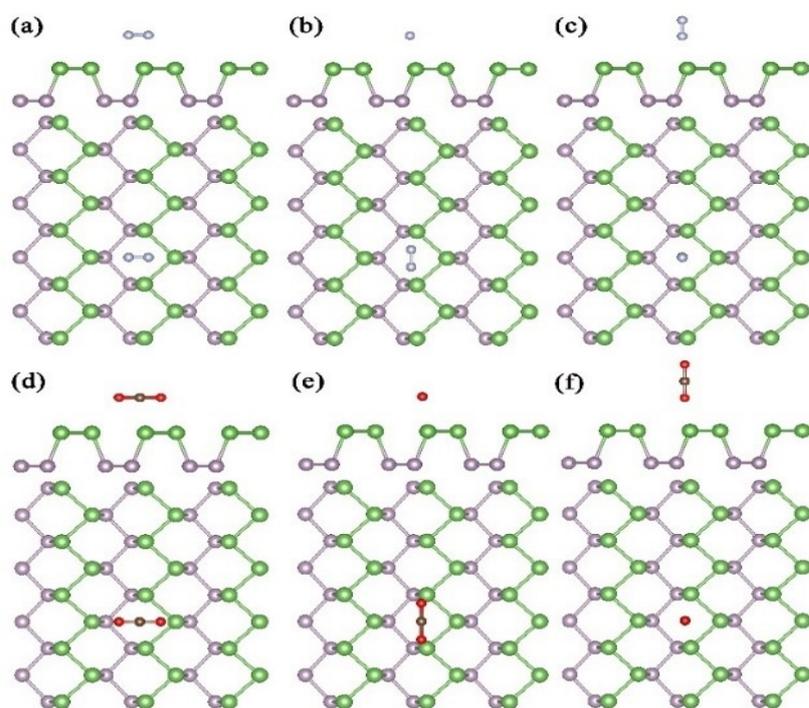


Figure S1 Initial adsorption configurations of (a–c) N_2 and (d–f) CO_2 molecules on the As surface of the Janus AsP monolayer. Purple, green, blue, red, and brown spheres represent P, As, N, O, and C atoms, respectively.

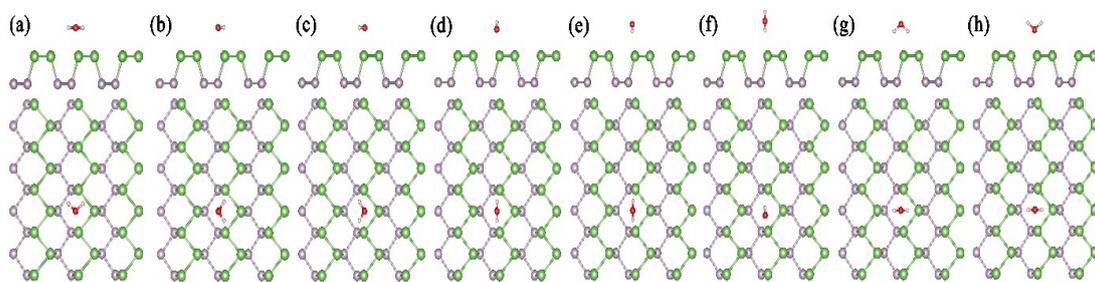


Figure S2. Initial adsorption configurations of H_2O molecules on the As surface of the Janus AsP monolayer. Purple, green, red, and white spheres represent P, As, O, and H atoms, respectively.

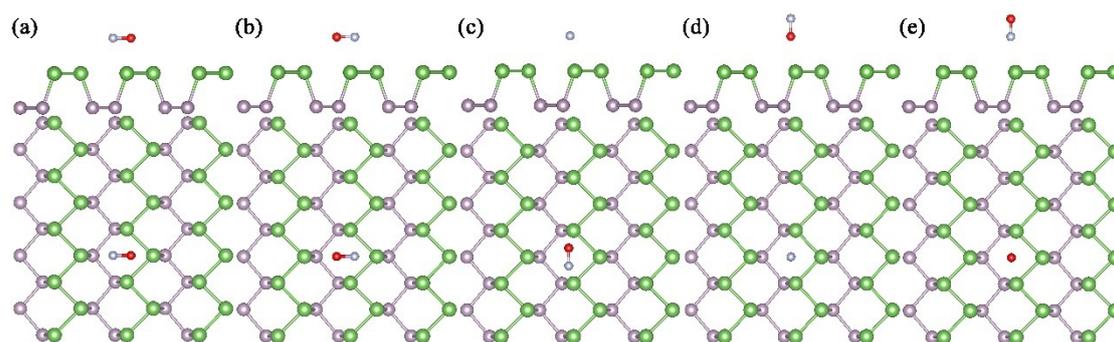


Figure S3. Initial adsorption configurations of NO molecules on the As surface of the Janus AsP monolayer. Purple, green, blue, and red spheres represent P, As, N, and O atoms, respectively.

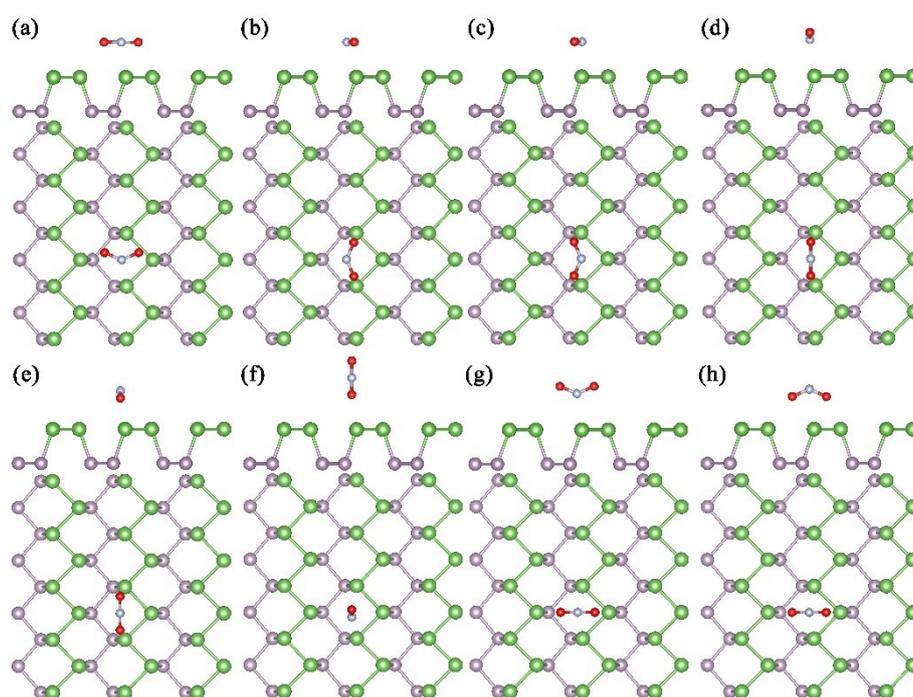


Figure S4. Initial adsorption configurations of NO_2 molecules on the As surface of the Janus AsP monolayer. Purple, green, blue, and red spheres represent P, As, N, and O atoms, respectively.

AsP-N₂

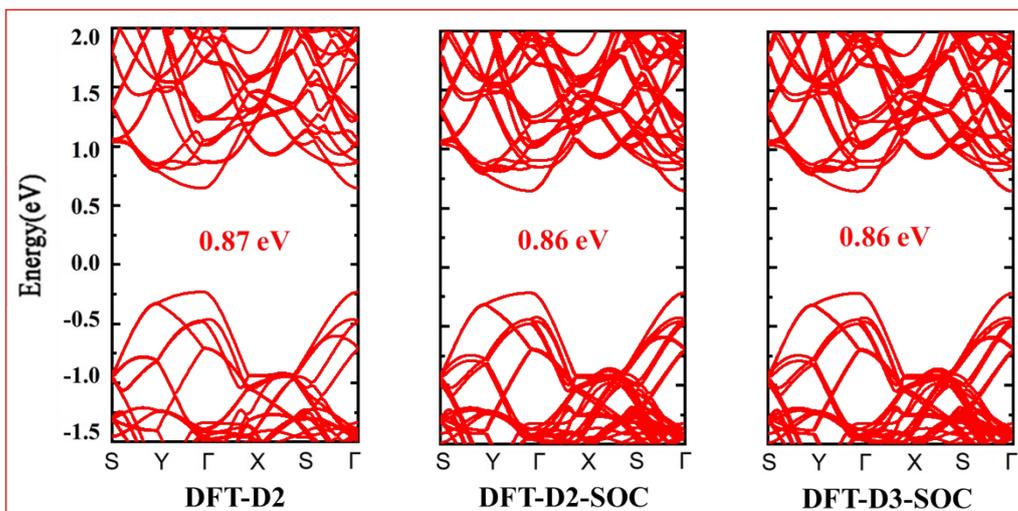


Figure S5. Band structures of AsP-N₂ adsorption systems calculated using the PBE functional with DFT-D2, DFT-D2-SOC (spin orbit coupling effect), and DFT-D3-SOC corrections, respectively.

AsP-H₂O

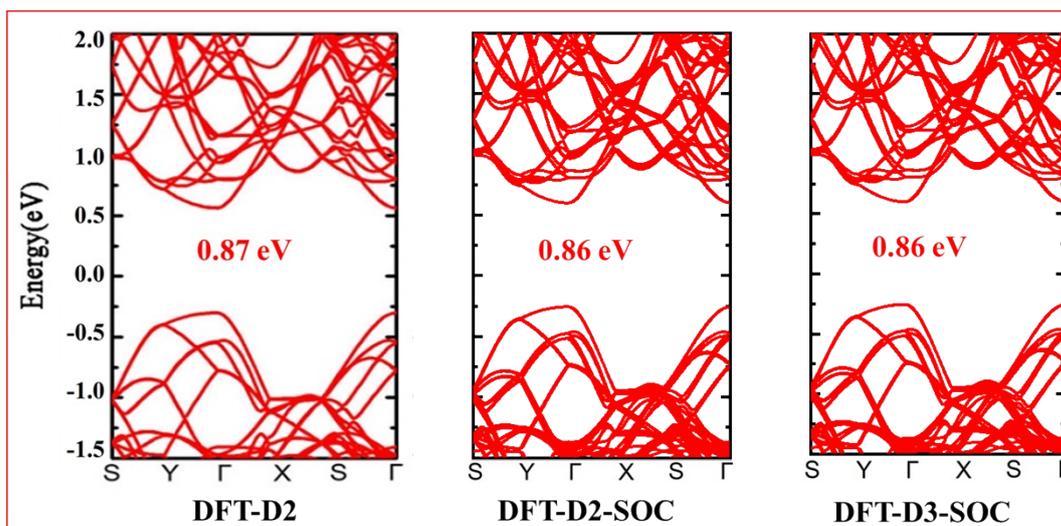


Figure S6. Band structures of AsP-H₂O adsorption systems calculated using the PBE functional with DFT-D2, DFT-D2-SOC (spin orbit coupling effect), and DFT-D3-SOC corrections, respectively.

AsP-CO₂

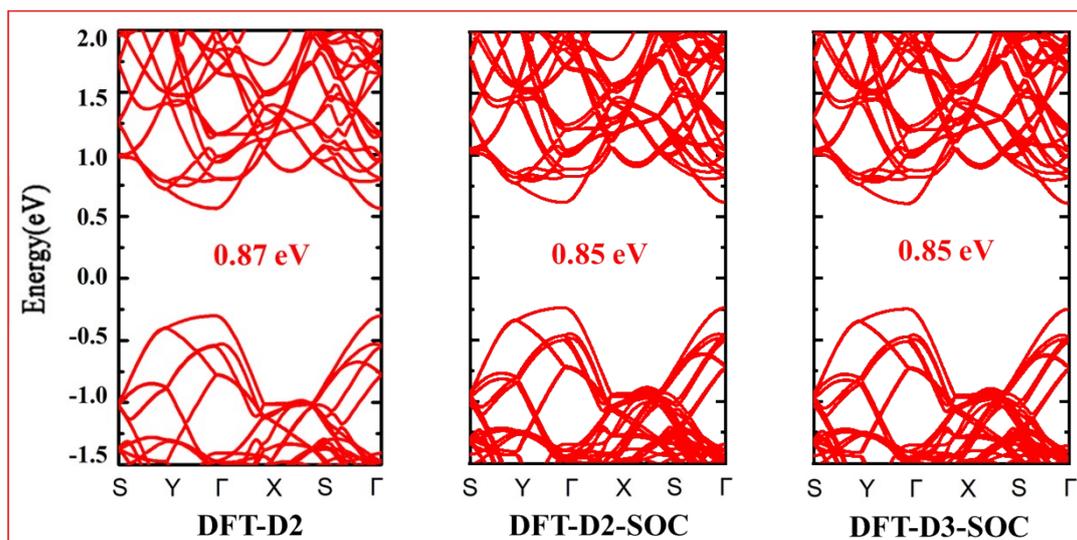


Figure S7. Band structures of AsP-CO₂ adsorption systems calculated using the PBE functional with DFT-D2, DFT-D2-SOC (spin orbit coupling effect), and DFT-D3-SOC corrections, respectively.

AsP-NO

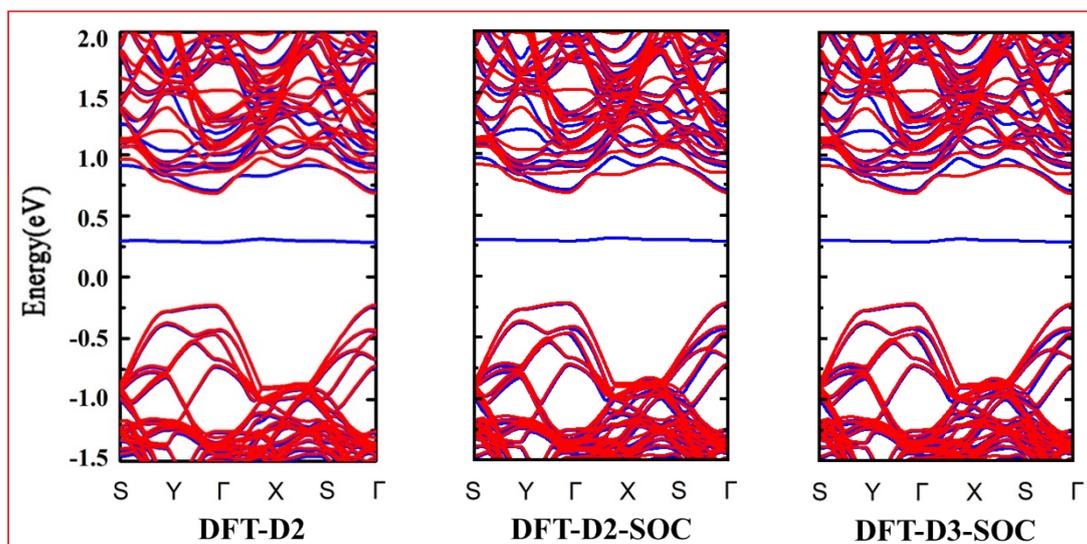


Figure S8. Band structures of AsP-NO adsorption systems calculated using the PBE functional with DFT-D2, DFT-D2-SOC (spin orbit coupling effect), and DFT-D3-SOC corrections, respectively.

AsP-NO₂

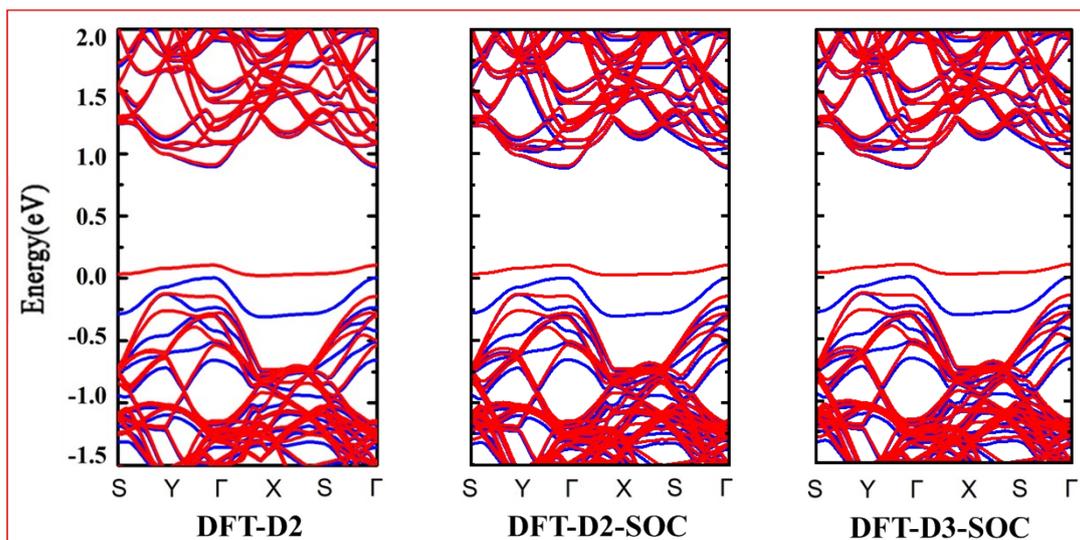


Figure S9. Band structures of AsP-NO₂ adsorption systems calculated using the PBE functional with DFT-D2, DFT-D2-SOC (spin orbit coupling effect), and DFT-D3-SOC corrections, respectively.

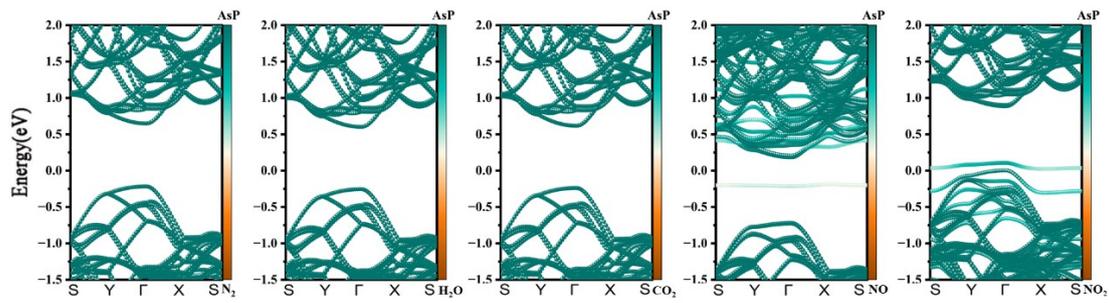


Figure S10. Projected band structures of different adsorption systems calculated using the PBE functional with DFT-D2 corrections.

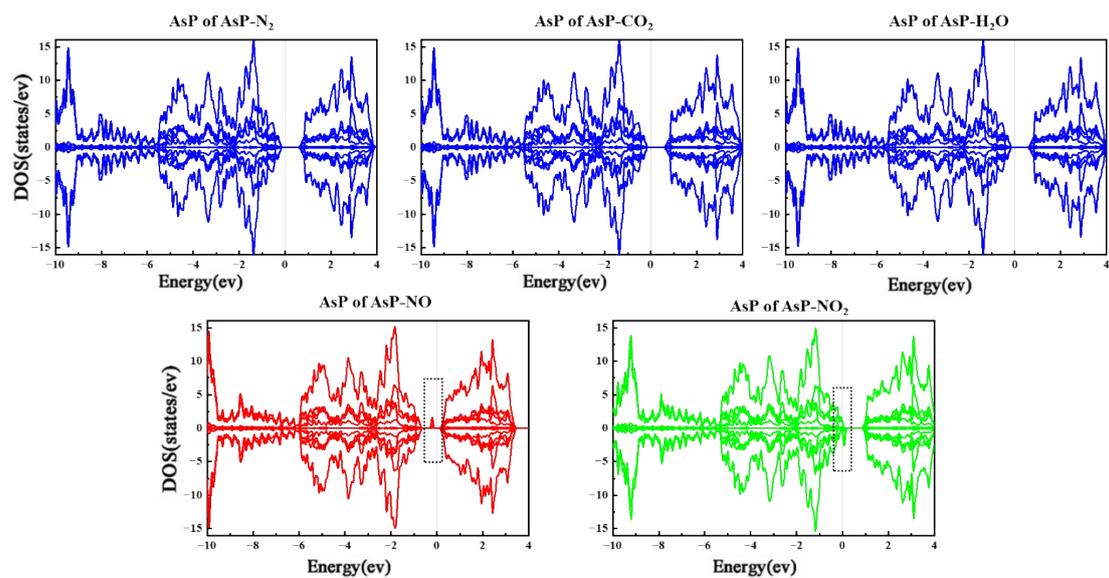


Figure S11. DOS of AsP of different AsP-gas adsorption systems. The black boxes highlight the asymmetric states, and the gray line denotes the Fermi level.

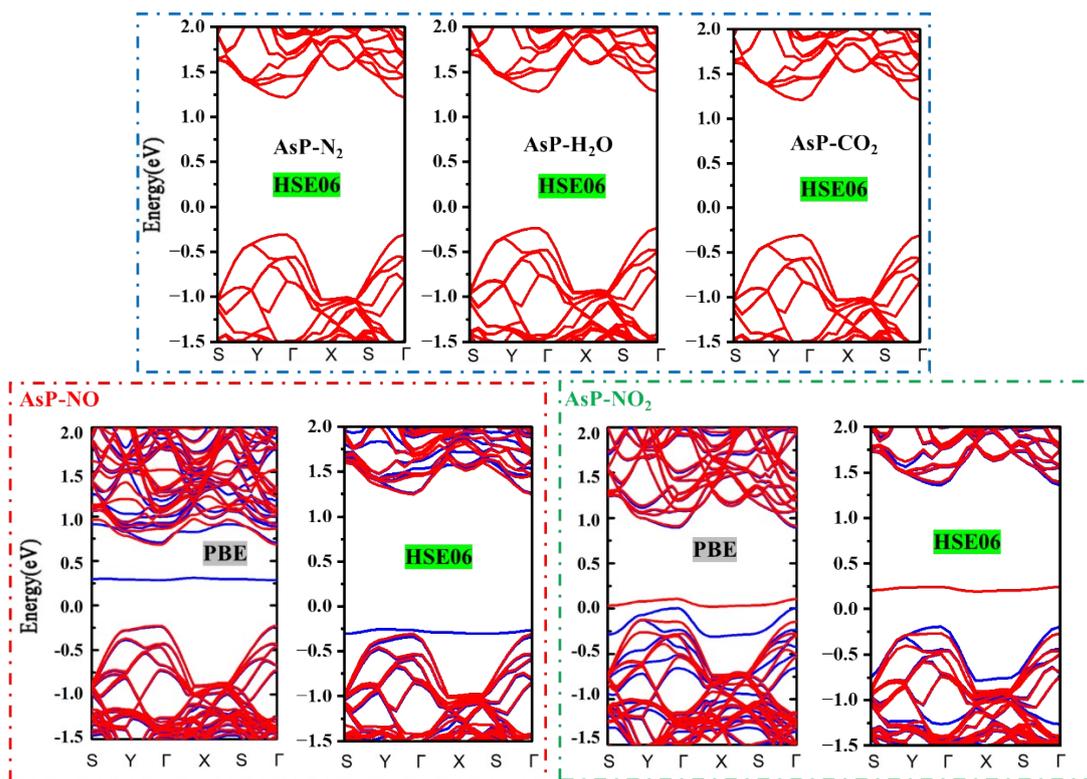


Figure S12. Band structures of different adsorption systems calculated using the PBE or HSE06 functional.

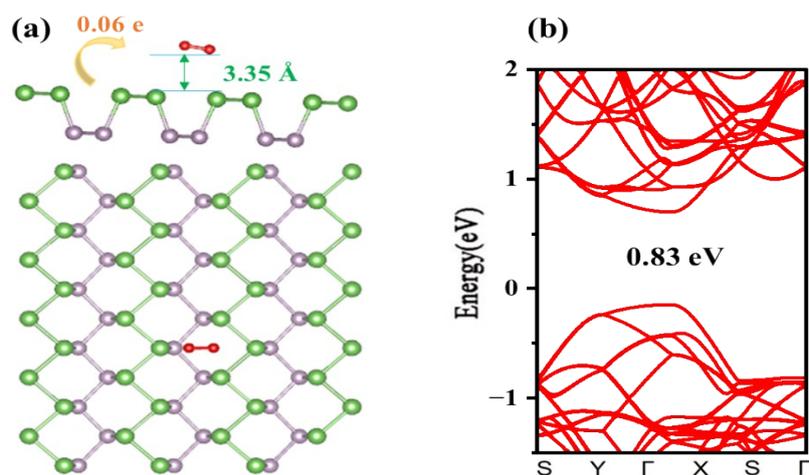


Figure S13. (a) The most stable adsorption configuration of O_2 molecules on the Janus AsP monolayer. Purple, green, and red pellets represent P, As, and O atoms, respectively. The annotated labels indicate the gas–surface adsorption distances and the associated charge-transfer values for each adsorption system. (b) Band structures of O_2 adsorption systems calculated using the PBE functional.

Table S1. -ICOHP of different adsorption systems.

Gas	N ₂	CO ₂	H ₂ O	NO	NO ₂
-ICOHP	-0.042	0.009	0.018	0.870	0.419