Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

A novel two-dimensional δ-InP_3 monolayer with high stability, tunable bandgaps, high carrier mobility and gas sensing of NO_2

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Table S1. Unit−cell parameters and atomic positions of δ-InP_3 monolayer.

Compounds	Space group	Lattice parameters(Å, °)	Atomic positions
δ-InP_3	*Pc*	a= 5.61; b= 21.26; c= 5.28; α=γ=90; β= 87.65	In (0.790 0.446 0.511) P1 (0.2670 0.550 0.952) P2 (0.694 0.429 0.006) P3 (0.304 0.553 0.531)

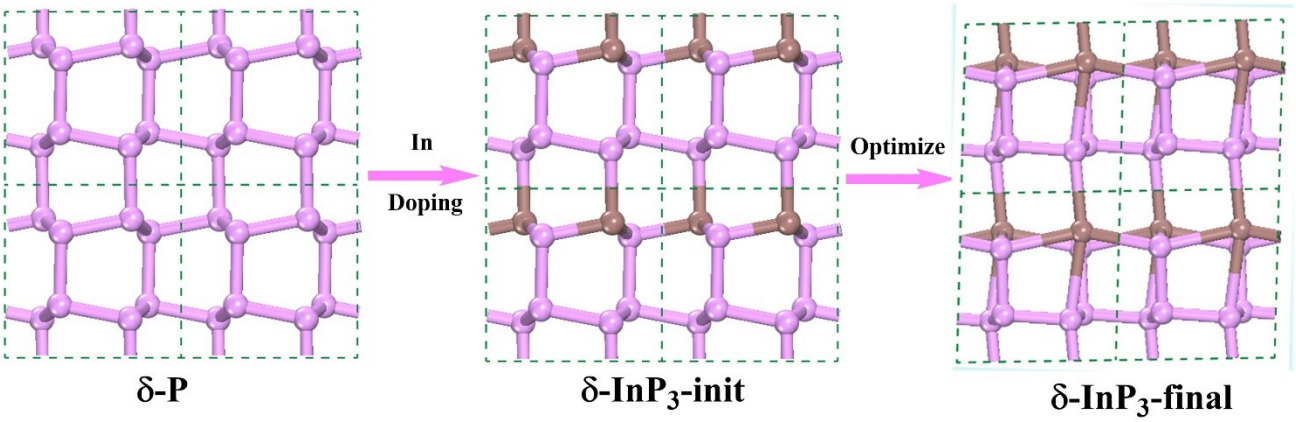

Figure S1 Doping progress of δ-InP_3 monolayer from δ-phosphorene.

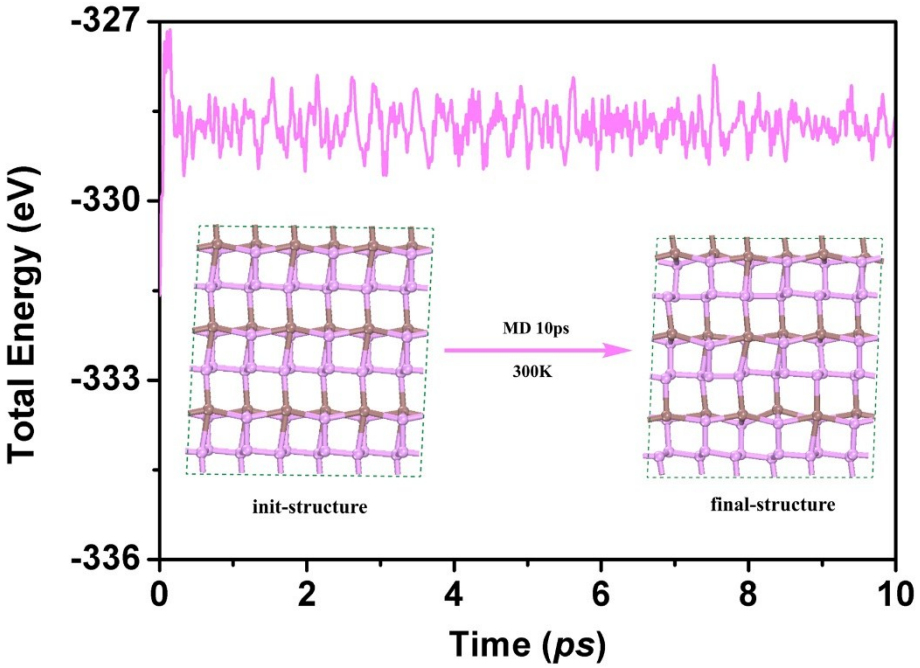

Figure S2 Evolution of total energy as a function of time step at 300K and snapshots of initial and final structure of δ-InP_3 monolayer in AIMD simulations at 0 and 10 ps.

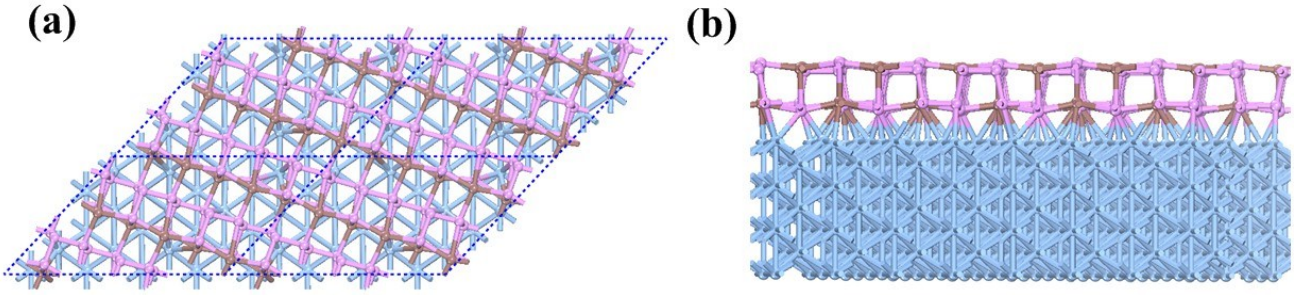

Figure S3 Top view (a) and side view (b) of the optimized δ-InP_3 monolayer on Ag (110) substrate. The unit cell is a $\sqrt{10} \times \sqrt{5}$ supercell of δ-phosphorene on a $4 \times \sqrt{13}$ supercell of Ag (110) substrate, with lattice mismatch of 0.54%.