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-InP₃ monolayer.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Space group</th>
<th>Lattice parameters(Å, °)</th>
<th>Atomic positions</th>
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</thead>
<tbody>
<tr>
<td>δ-InP₃</td>
<td>Pc</td>
<td>$a= 5.61; b= 21.26;$ $c= 5.28;$ $\alpha=\gamma=90; \beta= 87.65$</td>
<td>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)</td>
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Figure S1 Doping progress of δ-InP₃ 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 $\delta$-InP$_3$ monolayer in AIMD simulations at 0 and 10 ps.

Figure S3 Top view (a) and side view (b) of the optimized $\delta$-InP$_3$ monolayer on Ag (110) substrate. The unit cell is a $\sqrt{10} \times \sqrt{5}$ supercell of $\delta$-phosphorene on a $4 \times \sqrt{13}$ supercell of Ag (110) substrate, with lattice mismatch of 0.54%.