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

Supporting Information

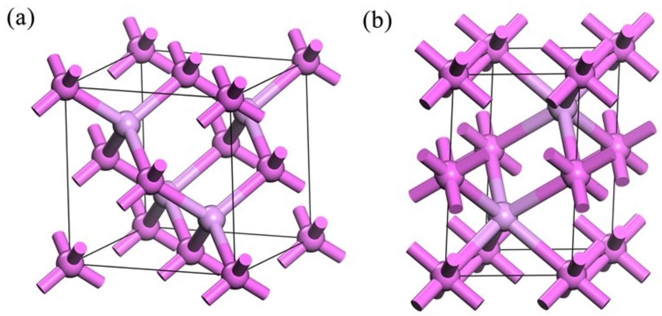

Figure S1. Bulk AlP with two different structure types: (a) ZnS and (b) NiAs prototype.

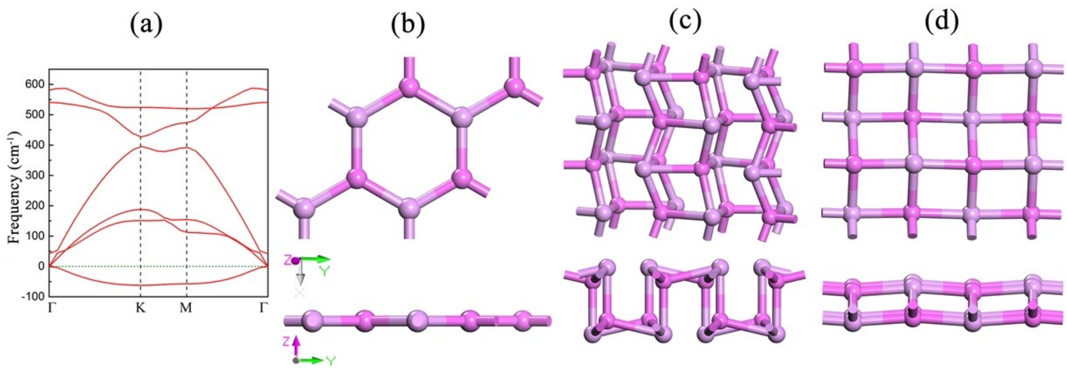

Figure S2. (a) phonon spectra of planar(hexagonal) AlP monolayer; Top-view and side-views from two horizontal directions for optimized structure of (b) hexagonal -AlP, (c) buckled-AlP, (d) puckered-AlP monolayer.

In-plane stiffness calculation method

The in-plane stiffness (C) is defined as $C = \left[\partial E / \partial \delta^2\right] / S_0$, in which E is the total energy, δ stands for the applied uniaxial strain and S_0 is the area of the optimized structure. To compute the in-plane stiffness (C) , we dilate the lattice of the cell up to 1.5% and the total energy – deformation is shown in Figure S2 (a).

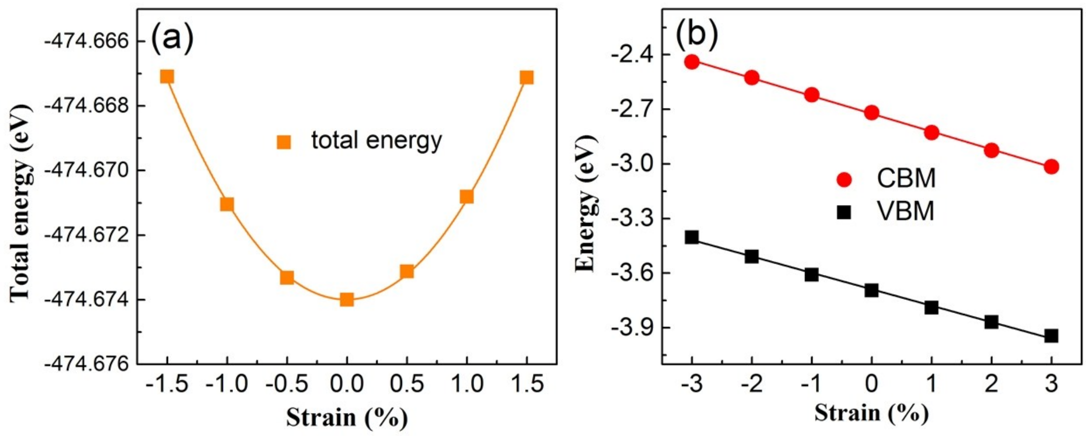

Figure S3. (a) The relations of the total energy to the applied strain. (b) Shifts of VBM and CBM under axial strain for *t*-AlP.

Carrier mobility

The acoustic-phonon-limited carrier mobility (μ) can be calculated using the following equation:

$$\mu = \frac{2e\hbar^3 C_{2D}}{3k_B T (m^*)^2 (E_1)^2}$$

The in-plane stiffness C_{2D} is given as the ratio between the second derivative of total energy with respect to axial strain and the equilibrium area of structure [Fig. S2 (a)]. The carrier effective mass along the transport direction is calculated using the equation $m^* = \hbar^2(\partial^2 E/\partial k^2)^{-1}$. The deformation potential constant E_1 of electron (hole) is defined as the rate of the conduction (valence) band edge position difference as the positions of band edges with respect to the axial tension and compression [Fig. S2 (b)]. Both the positions of CBM and VBM decrease monotonously while the strain increasing resulting a deformation potential constant of −9.88 eV (for electron) and −8.99 eV (for hole), respectively.

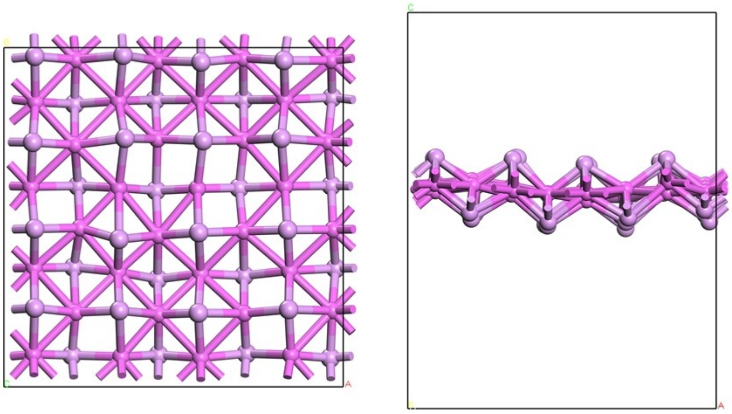

Figure S4. The snapshot of the final frame for the molecular dynamics simulation at 1200 K.

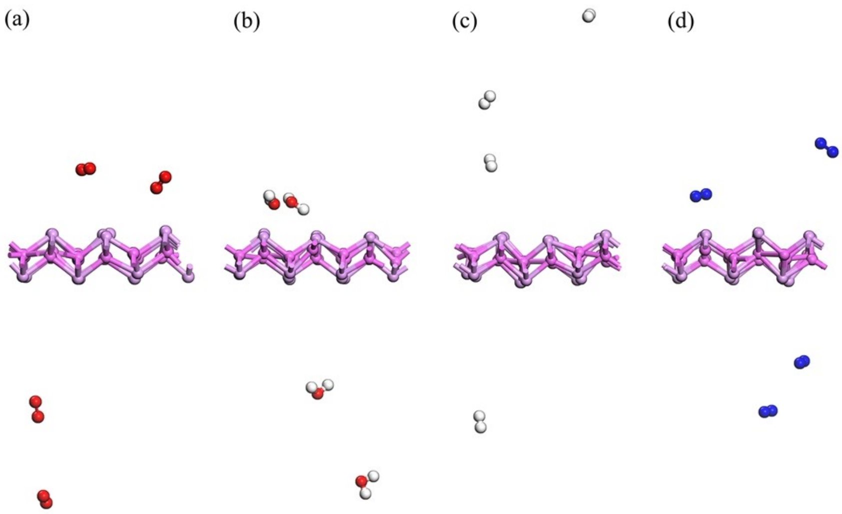

Figure S5. *Ab initio* MD snapshots of the *t*-AlP 3×3 supercell structures exposed to the high pressure (a) oxygen gas, (b) water vapour, (c) hydrogen gas and (d) nitrogen gas at temperatures T=1000K.