Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Material:

"Phosphorene Oxide: Stability and electronic properties of a novel 2D material"

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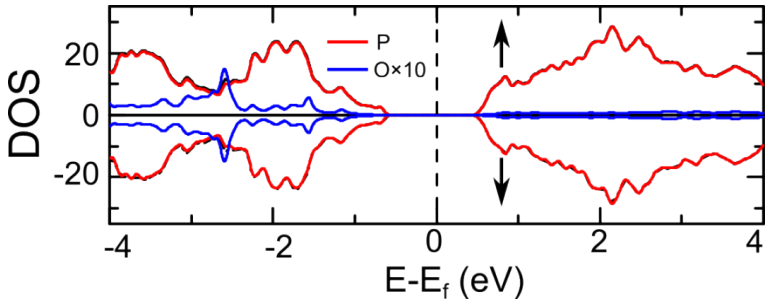

Figure S1. Density of states with a single oxygen adsorbed on phosphorene.

In the equilibrium configuration (Figure S2), O_2 binds to a phosphorus atom (P1) with a tilt configuration where $R_{(P1\text{-}O1)}$ = 1.69 Å and $R_{(P1\text{-}O2)}$ = 1.75 Å. As seen from the side view, O1 is closer to the surface with the distance of *d*=1.03 Å whereas O2 is far away with from the surface with the distance of about 1.75 Å. Therefore, O2 was moved laterally to determine the dissociation energy. A lateral displacement of O1 atom while fixing O2 atom will lead to a higher energy barrier since the distance of O1 from the top P atoms is only 1.03 Å.

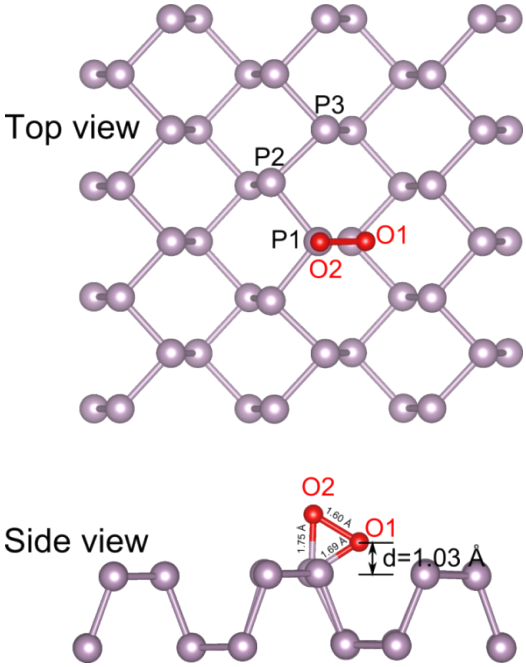

Figure S2. The top and side views of an oxygen molecule adsorbed on the phosphorene surface.

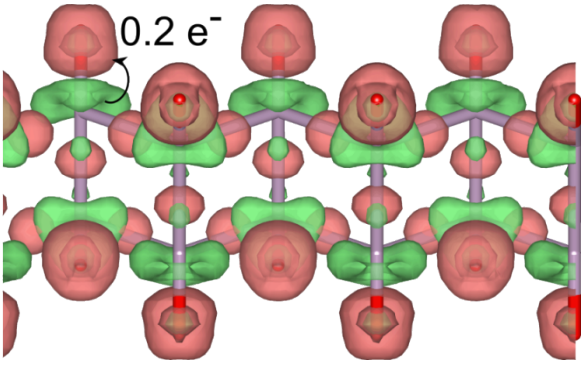

Figure S3. Deformation charge density of phosphorene oxide. The red region represents the accumulation of electrons and green region represents the depletion of electrons.

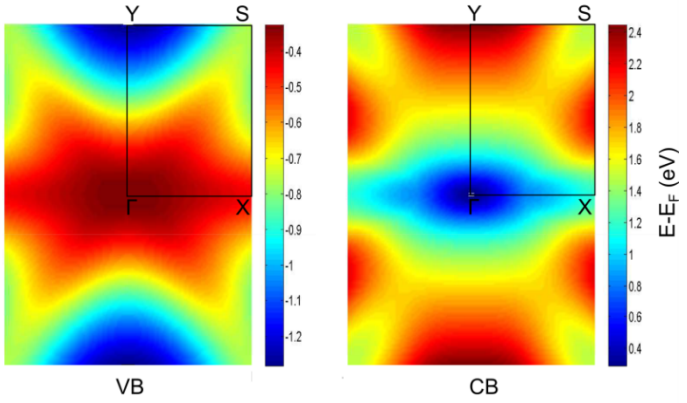

Figure S4. Two dimensional band structure of phosphorene oxide: (a) valence band, (b) conduction band.

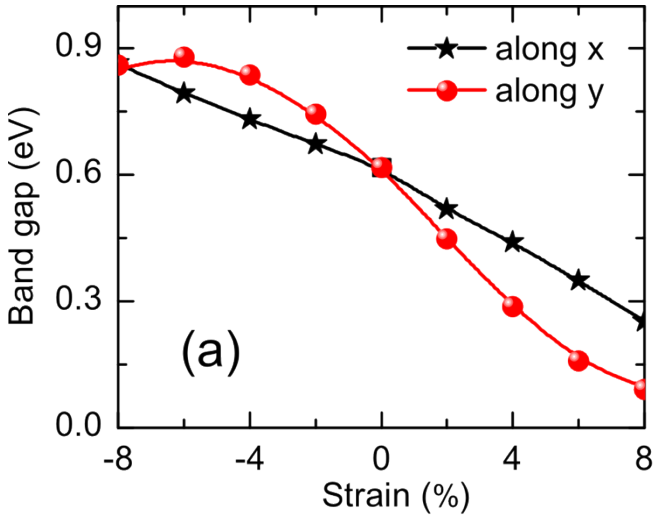

Figure S5. In-plane compressive and tensile strain effect on the band gap of phosphorene oxide.

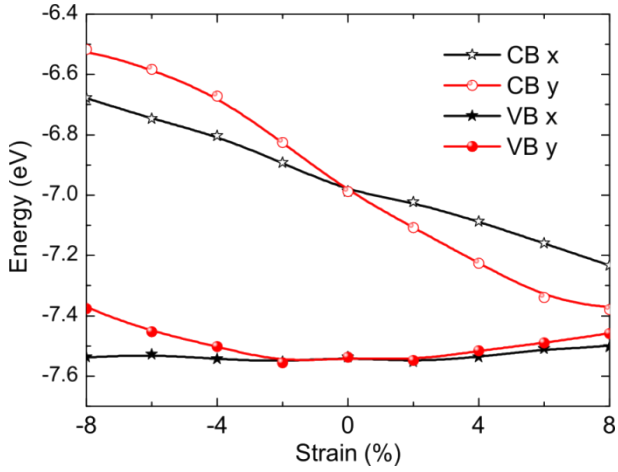

Figure S6. Phosphorene oxide: variation of valence and conduction bands at Γ point with strain along x (black) and y (red) directions: top of the valence band (solid dots) and bottom of the conductive band (open dots)

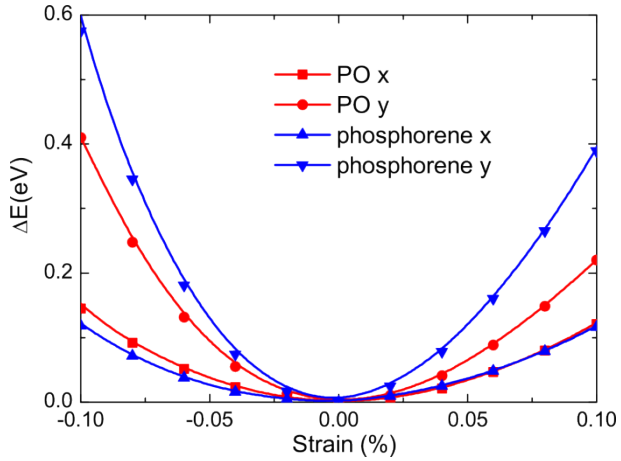

Figure S7. Variation of energy with strain for phosphorene and phosphorene oxide.

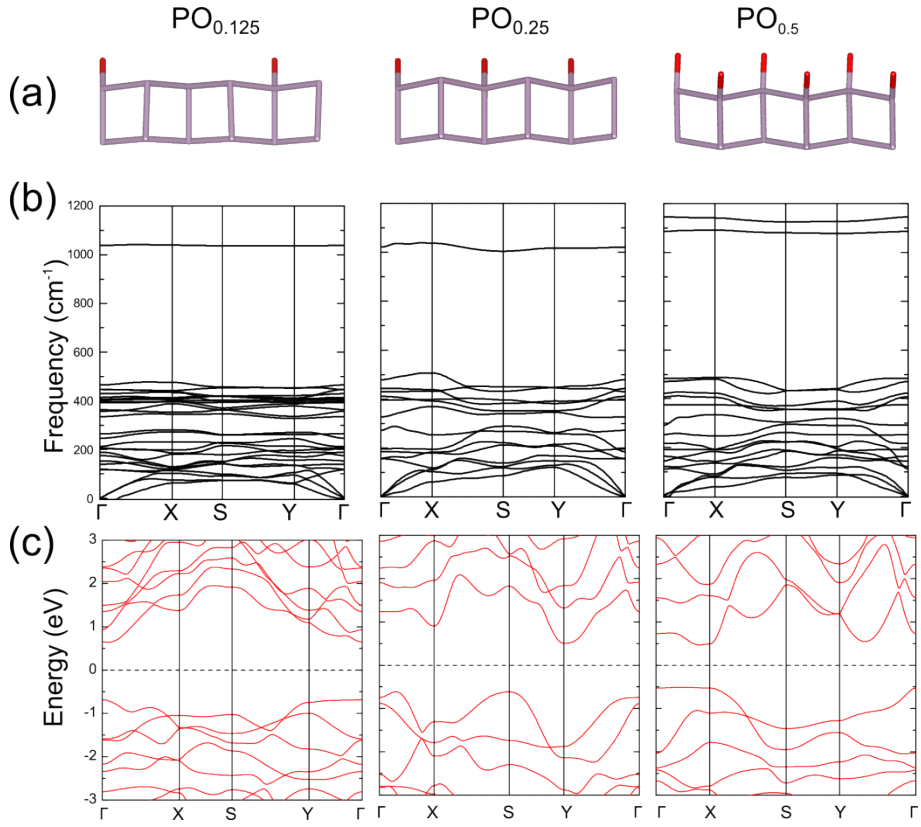

Figure S8. (a) Structure, (b) phonon dispersion curves, and (c) band structures for $PO_{0.125}$, $PO_{0.25}$, and $PO_{0.5}$. The direct band gap is defined as the energy gap at Γ. The indirect band gap is defined as (Γ→Γ-X), (S→Y), and (Γ →Γ-X), and (Γ→Γ-X) for $PO_{0.125}$, $PO_{0.25}$, $PO_{0.5}$, respectively. Γ, S, Y and X are defined as (0,0,0), (1/2,1/2,0), (0,1/2,0), and (1/2,0,0), respectively.

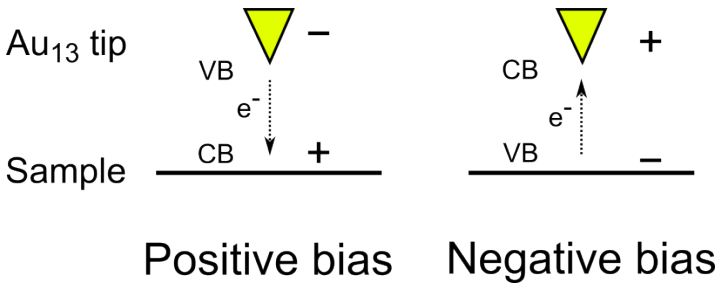

Figure S9. Schematic illustration of the STM set up.