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Supplementary

Red phosphorus in its two-dimension limit: novel clathrates with varying band gaps and superior chemical stabilities

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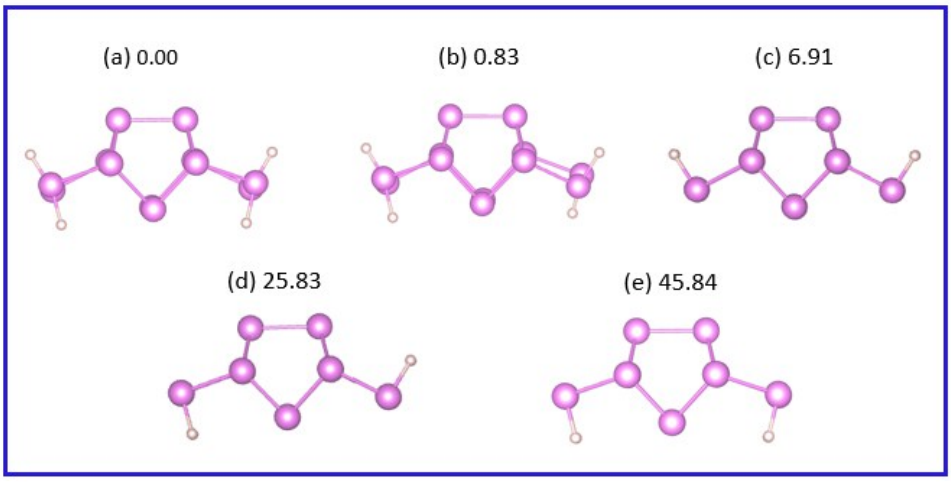

Figure S1. Geometric structures and relative energies (meV/atom) of $P_{12}H_4$ conformers optimized at PBE scheme.

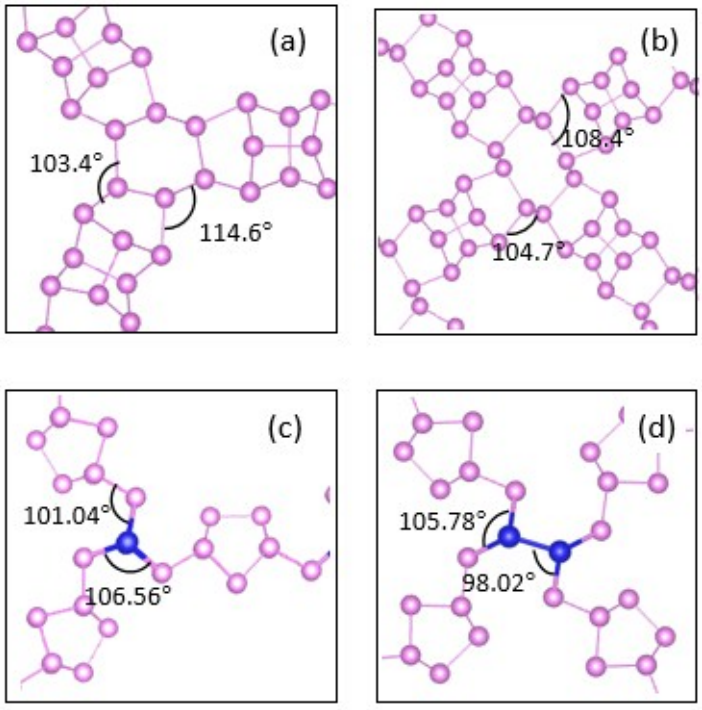

Figure S2. Bonding angles between P_{12} building blocks for (a) P-Hex, (b) P-Monoclinic, (c) V-Hex, and (d) V-Tetr, The bridge P atoms and P dimers are highlighted in blue.

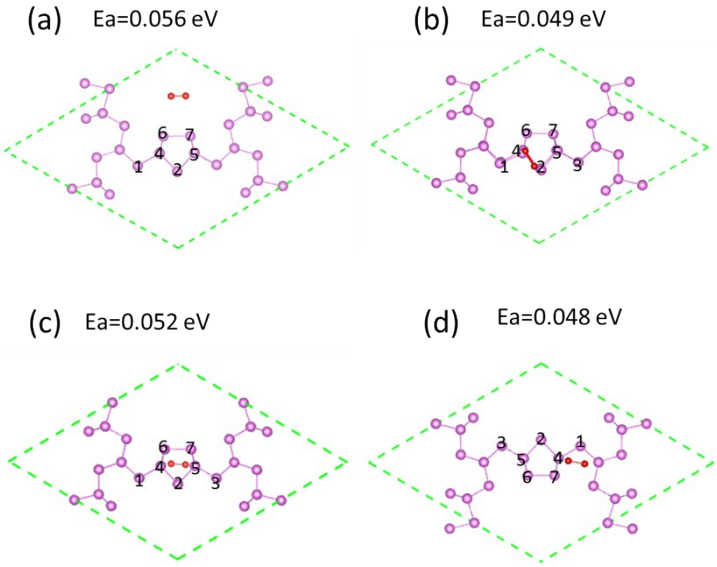

Figure. S3. Top view of the examined possible adsorption configurations of O_2 molecule adsorbed on allotrope of V-Hex. Ea denotes the adsorption energy per O_2 molecule. P and O atoms are colored in pink and red, respectively.

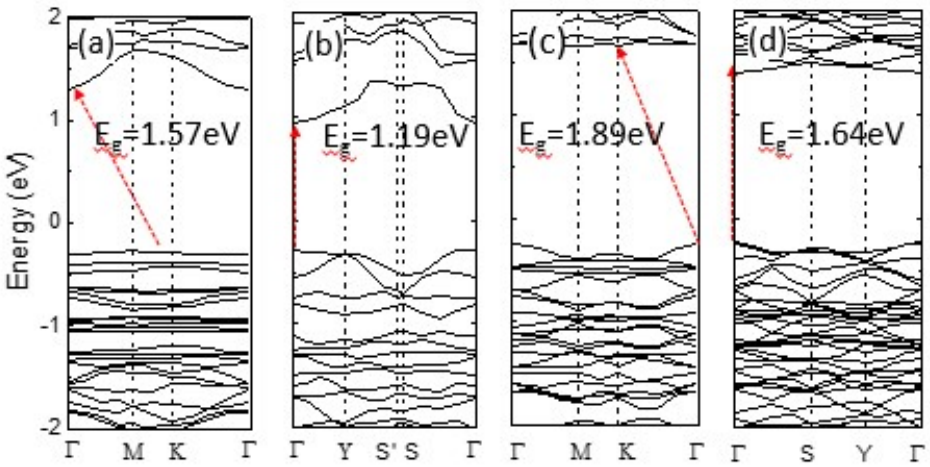

Figure S4. Band structures of the 2D clathrate phosphorenes obtained within the PBE scheme for (a) P-Hex, (b) P-Monoclinic, (c) V-Hex, and (d) V-Tetr, all based on the P_{12} building blocks.

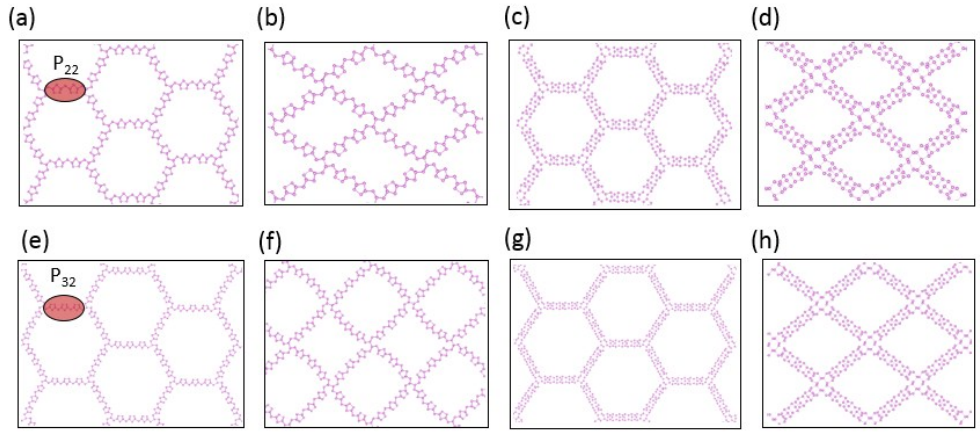

Figure S5. Geometric structures of V-Hex, V-Tetr, P-Hex, and P-Monoclinic formed with the P_{22} and P_{32} building blocks, respectively.

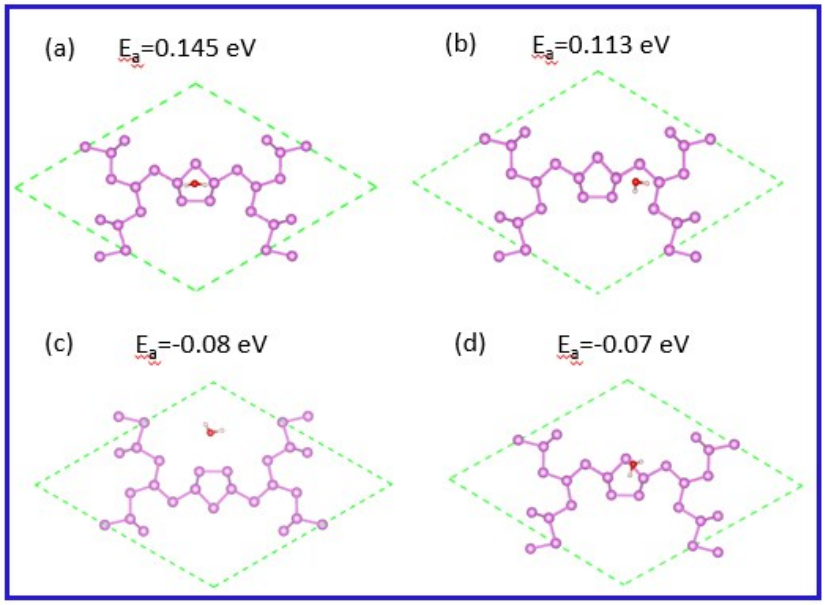

Figure S6. Top view of the examined possible adsorption configurations of H_2O molecule adsorbed on allotrope of V-Hex. E_a denotes the adsorption energy per H_2O molecule.

The following movies are evolutionary processes at the room temperature:

1. V-Hex-300K.mpg represents the V-Hex structure at T = 300 K in top view;

2. V-Tetr-300K.mpg represents the V-Tetr structure at T = 300 K in top view;

3. P-Hex-300K.mpg represents the P-Hex structure at T = 300 K in top view;

4. P-Monoclinic-300K.mpg represents the P-Monoclinic structure at T = 300 K in top view;

5. V-Hex-O_2.mpg represents the V-Hex exposed to O_2 at T = 300 K in top view.