Supporting Information

FeP_2 monolayer: Isoelectronic analogue of MoS_2 with excellent electronic and optical properties

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1. O_2 adsorption sites on the FeP_2 monolayer

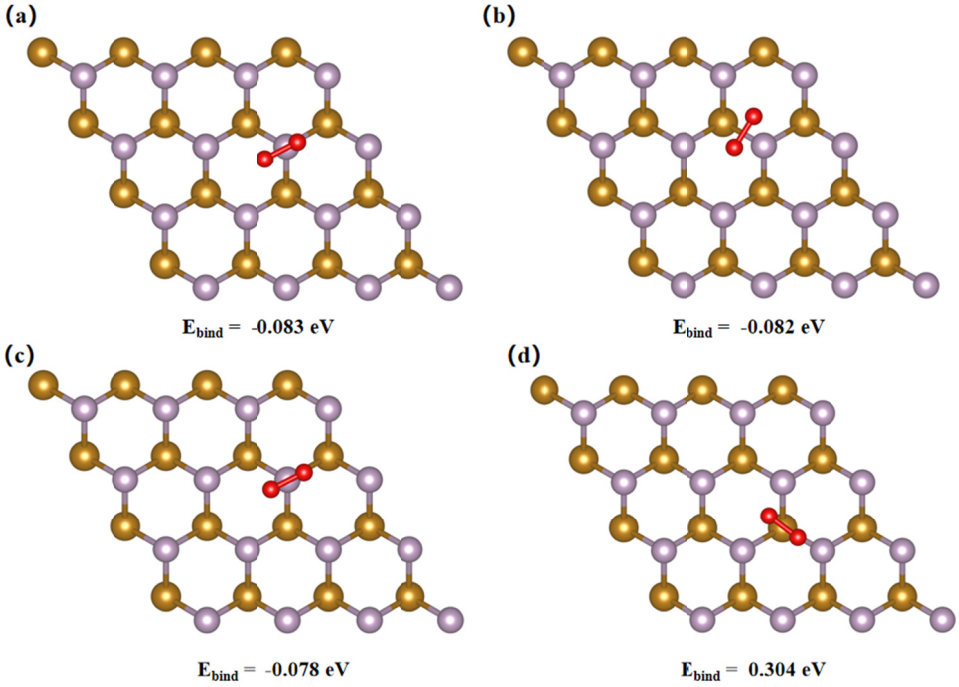

Fig. S1. Top view of several other adsorption sites for O_2 and the corresponding adsorption energies.

2. The oxidation resistance of the FeP_2 monolayer

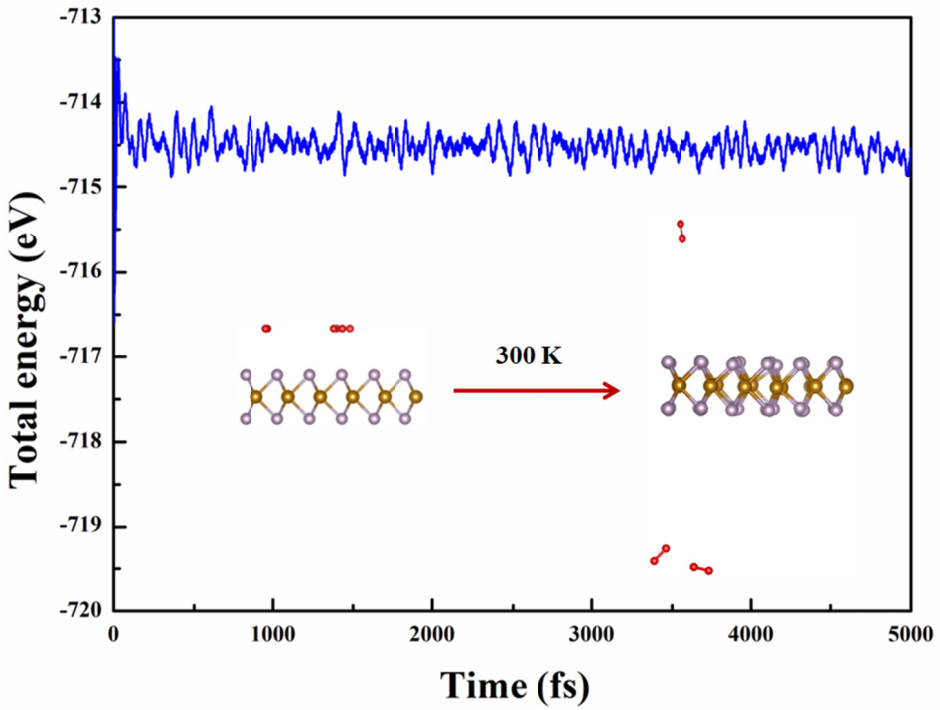

Fig. S2. Total energy and a snapshot of the FeP_2 monolayer with 3 O_2 molecules after a AIMD simulation of 5 ps at 300 K.

3. The band structure of K on the FeP_2 monolayer

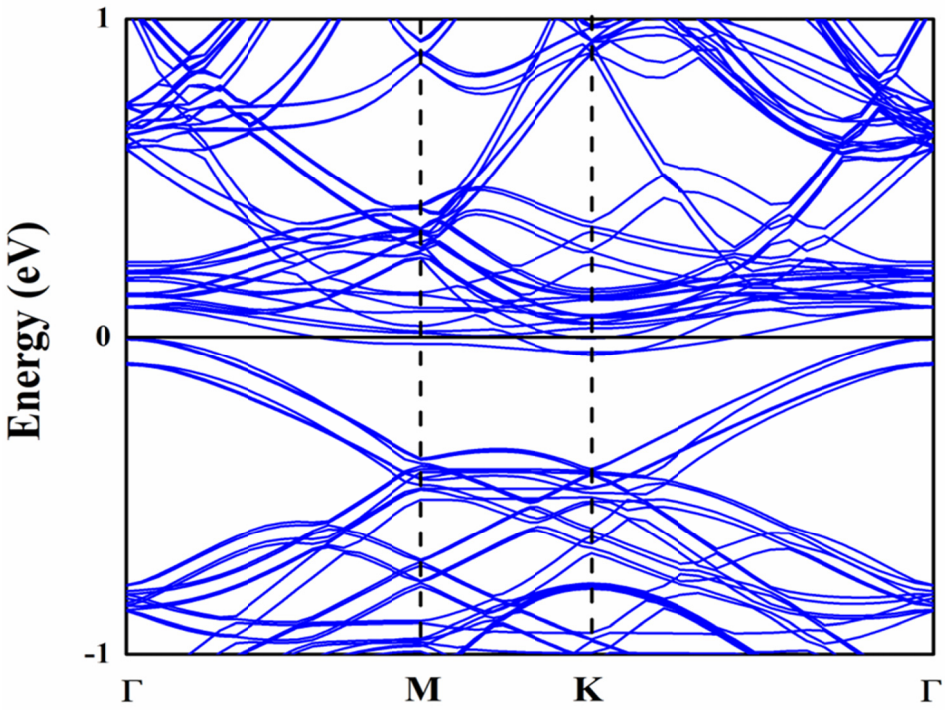

Fig. S3. Calculated band structure of 2D $Fe_{16}P_{32}K$ from PBE method.

4. The open circuit voltage profiles of K on the FeP_2 monolayer

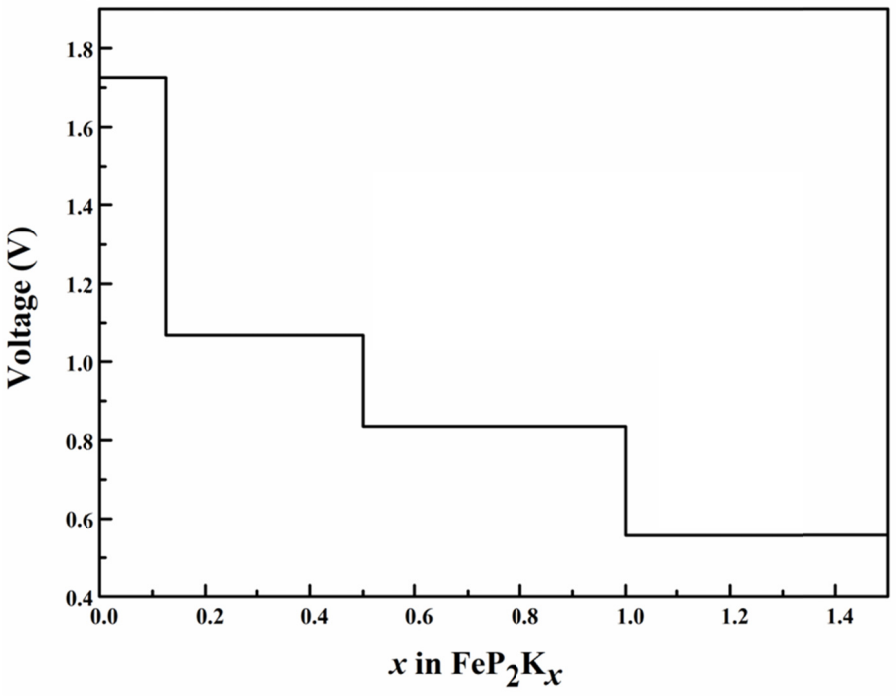

Fig. S4. Average voltages of different K concentrations in FeP_2K_x.

5. Thermal stability of the FeP_2 monolayer

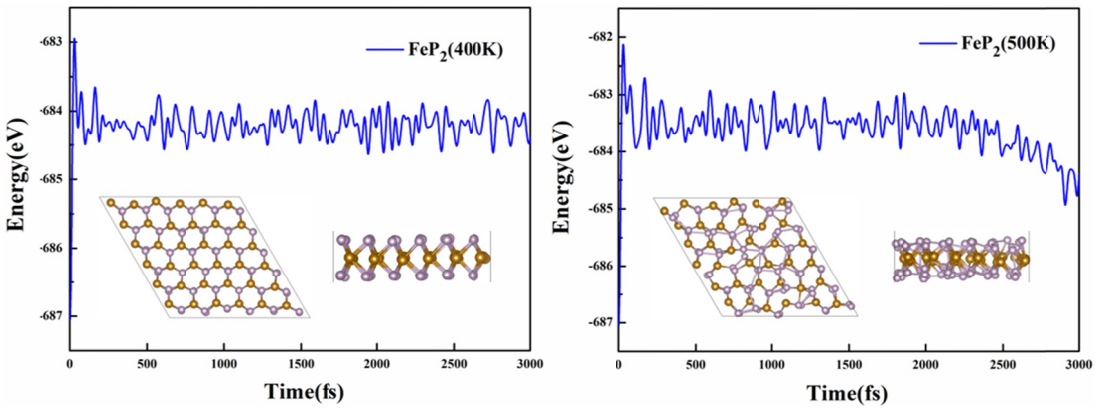

Fig. S5. AIMD simulation of the FeP_2 monolayer at 400 and 500 K, variation of energy fluctuation with time step and the snapshot of the FeP_2 monolayer.

6. Adsorption Energies on the FeP_2 monolayer

Table S1. Adsorption energies of various sites for K on the FeP_2 monolayer.

Site	A_1	A_2	A_3	A_4	A_5
E_{ad} (eV)	-1.78	-1.61	-1.76	A_1	A_1

7. Structural information of the FeP_2 monolayer

Table S2. Structural information of the predicted FeP_2 monolayer.

Lattice parameters(Å, °)		Wyckoff position, fractional coordinates		
		x	*y*	*z*
$a = b = 2.78$	Fe	0.33333	0.66667	0.50000
$c = 30$	P	0.66667	0.33333	0.55453
$\alpha = \beta = 90$	P	0.66667	0.33333	0.44547
$\gamma = 120$				

CONCAR

FeP_2

1.00000000000000

2.7799852124312334 0.0000000000000000 0.0000000000000000

-1.3899926062156167 2.4075378160654597 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

Fe P

1 2

Direct

0.3333333429999996 0.6666666870000029 0.5000000000000000

0.6666666870000029 0.3333333429999996 0.5545296792859190

0.6666666870000029 0.3333333429999996 0.4454703207140810