Supplementary Material

for

Selective Highly Sensitive Gas Sensors by BeP_2C Monolayer: A Theoretical Study

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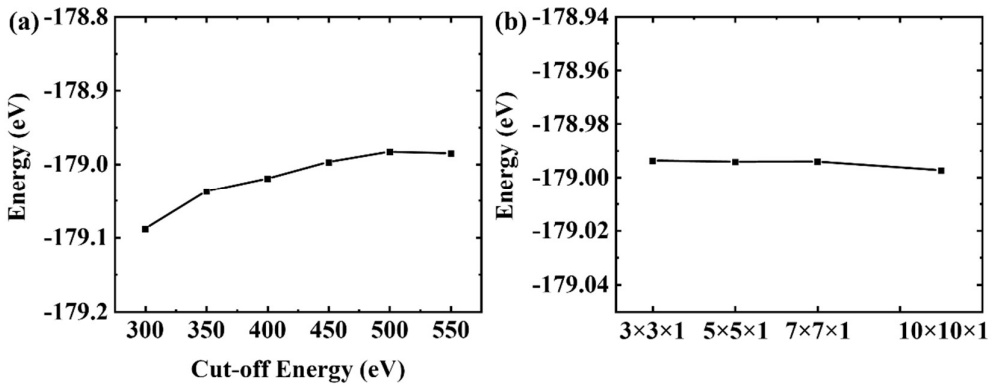

Fig. S1. Energy of the BeP_2C monolayer under (a)different cut-off energies and (b) different *k*-points.

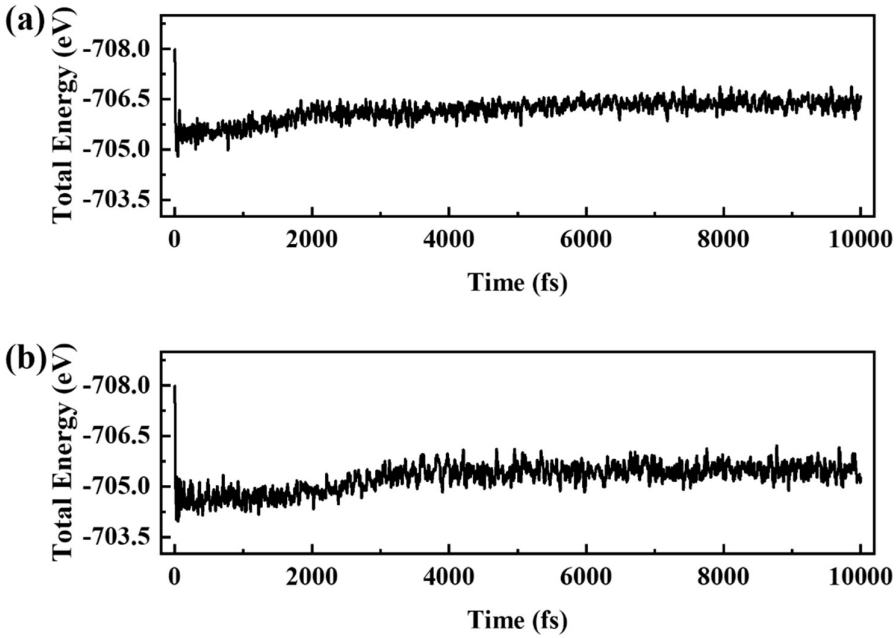

Fig. S2. The AIMD simulation of BeP_2C monolayer at (a) 300 K and (b) 400 K.

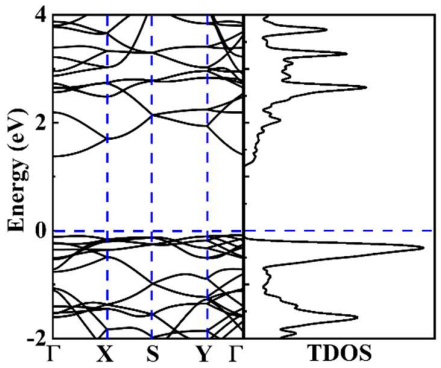

Fig. S3. The band structure and total density of states (TDOS) of BeP_2C monolayer of PBE methods.

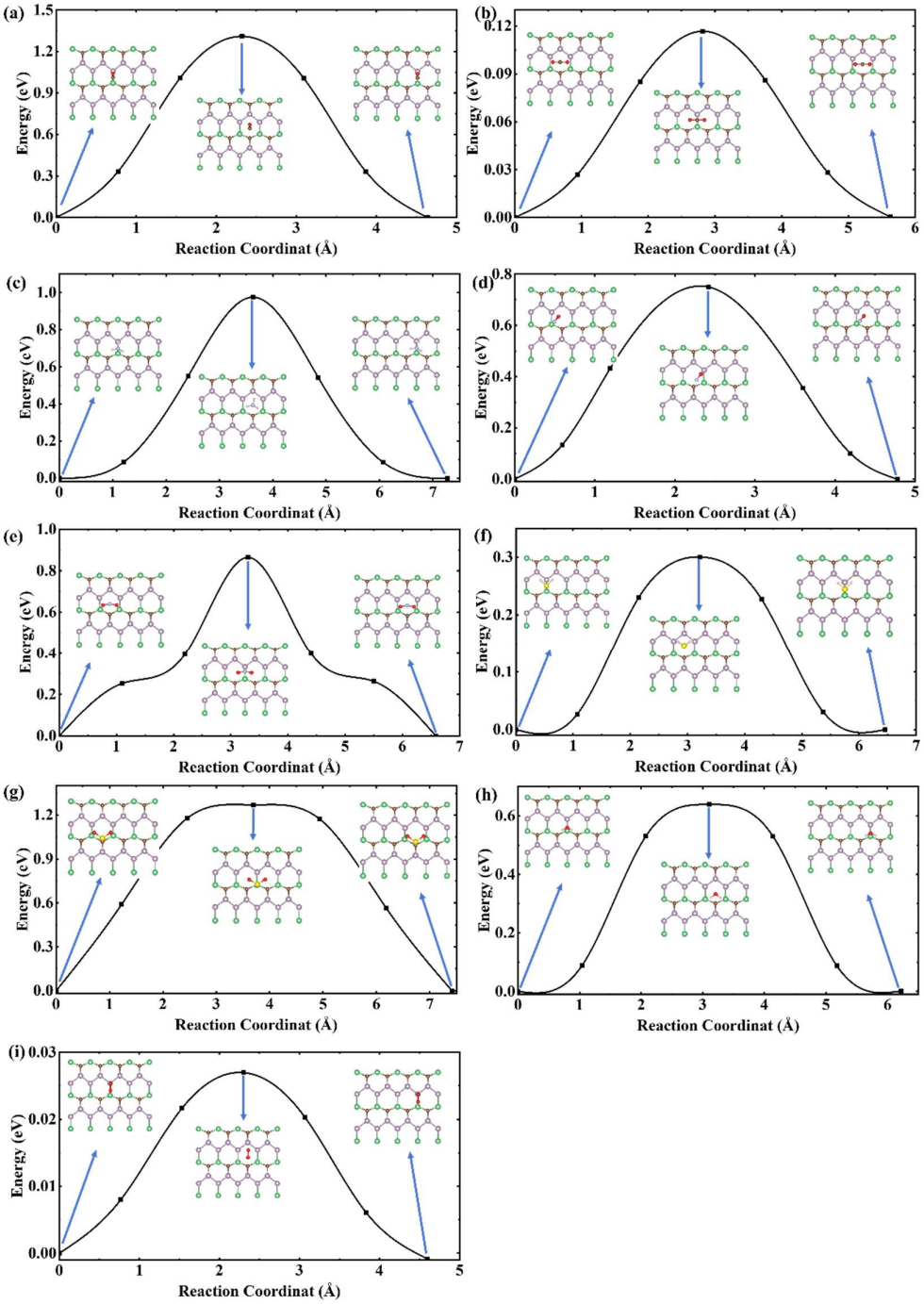

Fig. S4. Diffusion barriers of (a) CO, (b) CO_2, (c) NH_3, (d) NO, (e) NO_2, (f) H_2S, (g) SO_2, (h) H_2O, and (i) O_2 on the BeP_2C monolayer.

Table S1. Lattice and coordinate information of BeP_2C monolayer

a	b	c	
	3.250	5.500	20.000
	alpha	beta	gamma
	90.0	90.0	90.00
	x	y	z
Be	0	-0.043	-0.486
P1	0	0.322	-0.532
P2	0.5	0.547	-0.502
C	0.5	0.841	-0.485