Supplementary Information

An Ultra-Sensitive and Selective Nitrogen Dioxide Sensor Based on Novel P_2C_2 Monolayer from Theoretical Perspective

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Table S1. Comparison of the adsorption energy, equilibrium distance, and Mulliken charge transfer of NO_2 adsorbed on P_2C_2 monolayer (4×2 supercell, 11.67×16.36 Å^2) and black phosphorene (BP) monolayer (3×4 supercell, 9.95×17.59 Å^2 for our calculation; 3×3 supercell for Ref. 1 and Ref. 2). The E_a value of NO_2 adsorption on P_2C_2 monolayer is larger than that of NO_2 adsorption on BP, indicating that a higher level sensitivity for NO_2 detection with P_2C_2 monolayer than that with BP.

materials	E_a (eV)	d_0 (Å)	Q (e)	
P_2C_2	-1.318	2.02	0.117	This work
BP	-0.556	2.33	0.115	This work
BP	-0.50	2.27	0.185	Ref. [1]
BP	-0.62	2.2	-	Ref. [2]

Table S2. Comparison of the limit of detection (LOD), and sensitivity of NO_2 adsorbed on black phosphorene based sensors.

materials	LOD	sensitivity	
BP flakes	20 ppb	-	Ref. [3]
Multilayer BP	5 ppb	20% (20 ppb)	Ref. [4]
Multilayer BP	20 ppb	190% (20 ppb)	Ref. [5]

Table S3. Comparison of the adsorption energy (calculated by Eq. (1)), equilibrium distance, and Mulliken charge transfer of different

gas molecules adsorbed on P_2C_2 monolayer (4×2 supercell, 11.67×16.36 Å^2) and black phosphorene (BP) (3×3 supercell).

molecule	E_a (eV)			Q (e)			d_0 (Å)		
	This work(P_2C_2)	Ref.1	Ref.2	This work(P_2C_2)	Ref.1	Ref.2	This work(P_2C_2)	Ref.1	Ref.2
CO_2	-0.396	-	-0.41	-0.023	-	-0.04	3.09	-	2.69
H_2	-0.158	-0.13	-	0.018	-0.013	-	3.15	2.46	-
H_2O	-0.364	-0.14	-	-0.036	-0.035	-	3.16	2.71	-
N_2	-0.385	-	-	-0.017	-	-	3.16	-	-
NH_3	-0.483	-0.18	-0.50	-0.032	-0.050	-	3.19	2.59	2.14
O_2	-0.423	-0.27	-	-0.026	0.064	-	3.02	2.76	-
NO_2	-1.318	-0.50	-0.62	0.117	0.185	-	2.02	2.27	2.2

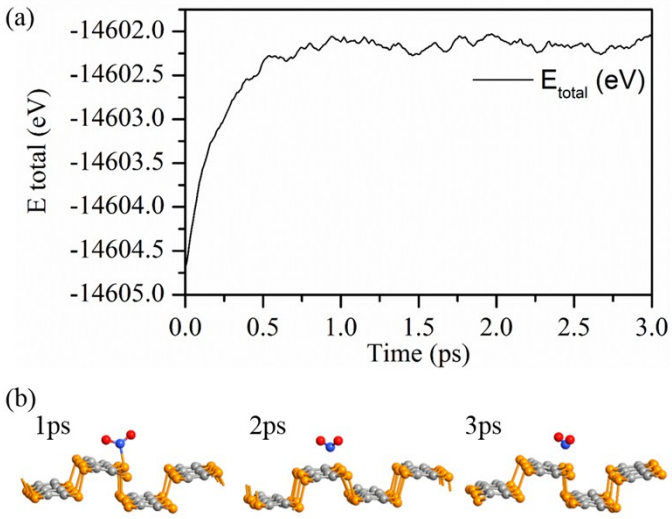

Fig S1. Molecular dynamics simulation results for NO_2-adsorbed P_2C_2 monolayers at T = 300 K. (a): total energy fluctuations with time; (b): structural configurations after 1ps, 2ps, and 3ps. We evaluated the thermal stability of NO_2-adsorbed systems at 300 K for 3 ps with a time step of 1 fs by performing the first-principle molecular dynamics (MD) simulations with the moles−volume−temperature (NVT) Berendsen ensemble.[6] It can be seen that the fluctuations of energy with time retain around a certain constant. Moreover, NO_2-adsorbed system does not suffer pronounced structural distortion or transformation, as shown in Fig. S1(b). Our calculation results reveal that NO_2-adsorbed P_2C_2 monolayer is thermally stable at room temperature.

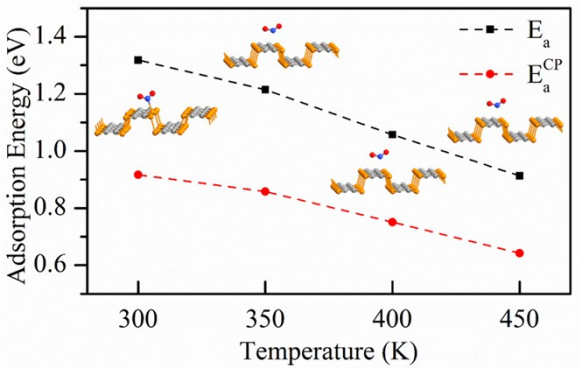

Fig S2. Adsorption energies of NO_2 adsorbed on monolayer P_2C_2 as a function of temperature.

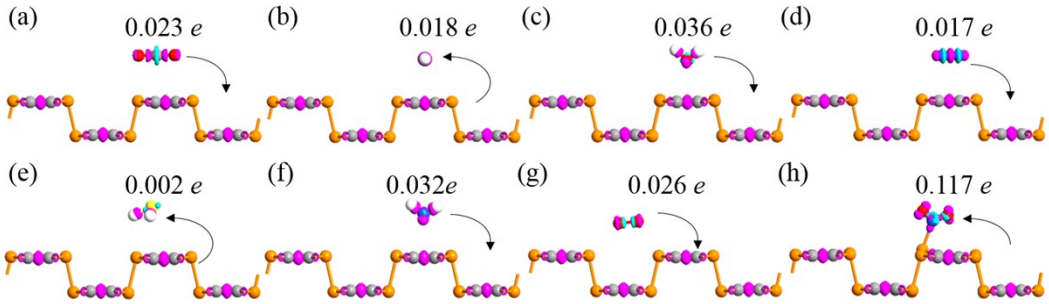

Fig S3. The side views of electron difference densities (EDD) calculation for (a) CO_2, (b) H_2, (c) H_2O, (d) N_2 (e) H_2S (f) NH_3, (g) O_2 and (h)NO_2 adsorbed on the P_2C_2 monolayer. The isovalue is 0.2 eV/Å^3. The direction of charge transfer is shown by the arrow.

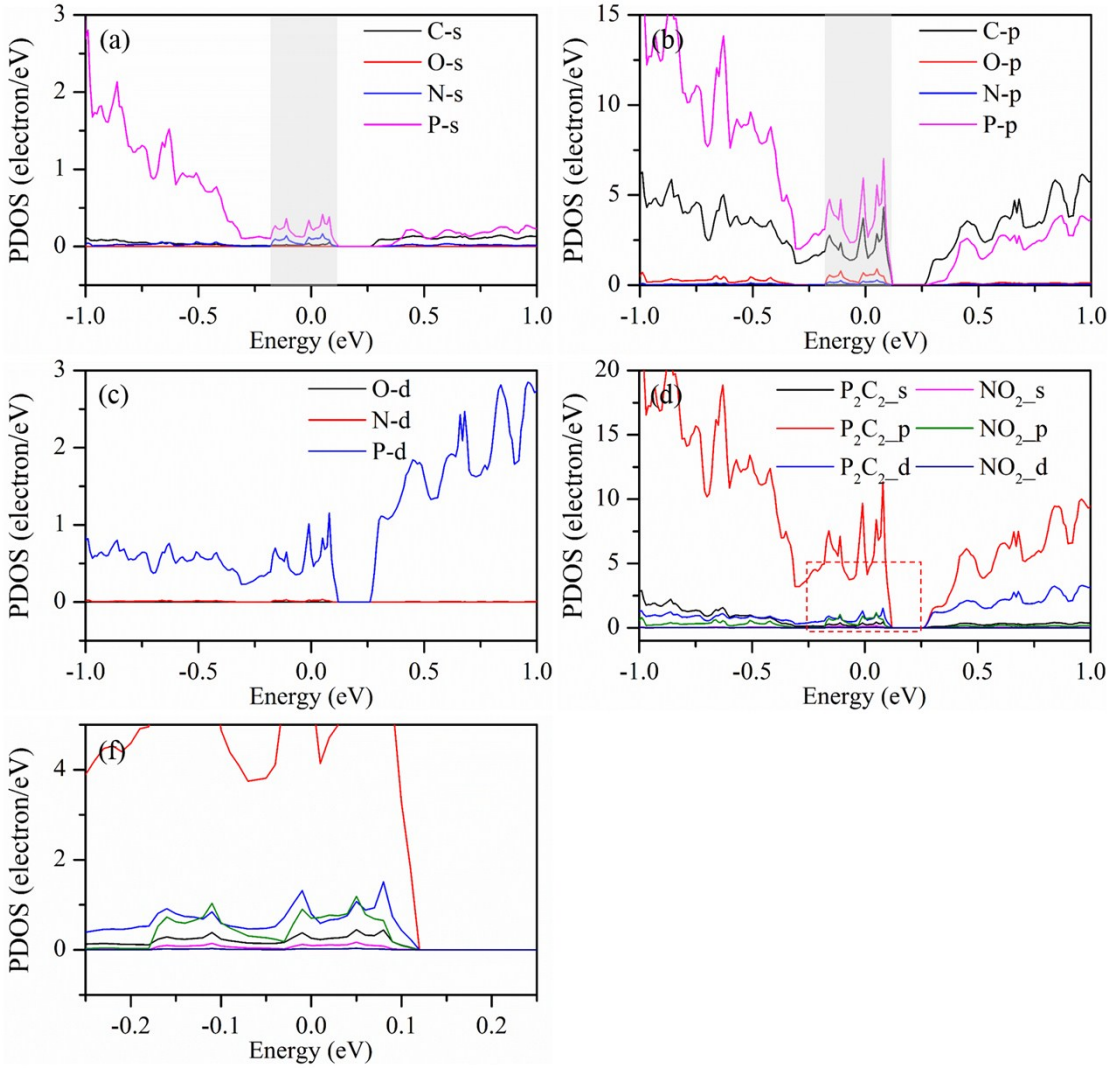

Fig S4. (a-f) The PDOS of NO_2 molecule adsorbed on P_2C_2 monolayer system. (f) is zoomed from (d) as indicated by red rectangle dotted line. The Fermi energy is set at zero.

References

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