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Supplementary Material

Carbon-Phosphide Monolayer with High Carrier Mobility and Perceptible I-V Response for Superior Gas Sensing

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1. VIBRATIONAL PROPERTIES

Table 1, shows the values of vibrational frequencies of isolated and absorbed gas molecules on the CP monolayer. The vibrational frequencies of gas molecules can thus be referred to judge the strength of the interactions. In case of CO with CP system, the stretching vibrational frequencies between C-O is found to be 2108.05 cm^{-1} which is red-shifted from it's isolated counterpart (2115.97 cm^{-1}),while in case of CO_2 molecule, there are two types of stretching occurs i.e., symmetric stretching and asymmetric stretching. The symmetric stretching of gas+CP system (isolated gas molecules) have lower vibrational frequencies 1313.00 cm^{-1} (1314.47 cm^{-1}) as compared to the asymmetric stretching with 2345.81 cm^{-1} (2353.09 cm^{-1}).Apart from this, it shows deformation vibrational frequencies in gas molecules absorbed on CP system which has $\approx$ 10 cm^{-1} lower than the isolated system.

For NH_3 molecule, the symmetric and asymmetric stretching of the gas-CP system (isolated gas) are 3365.15 cm^{-1} (3381.54 cm^{-1}) and 3512.88 cm^{-1} (3515.70 cm^{-1}), respectively. The above results clearly shows the weak interacting behaviour of three gases (CO, CO_2 and NH_3) that, we have already inferred from the binding energy and charge transfer calculations (refer main text).

Moreover, NO and NO_2 gas molecules interact strongly with CP system as both gases have higher binding energy and charge transfer. Also, from the vibration frequencies, we found significant changes for both the gases. The red-shift occurs when N-O bond stretch which changes from 1687.10 cm^{-1} for isolated to 1553.27 cm^{-1} in the absorbed case. In addition to that, we found asymmetric stretching in NO_2 i.e., 1479.32 cm^{-1} for isolated and 1495.33 cm^{-1} for absorbed case while symmetric stretching for isolated case was 1266.29 cm^{-1} and 1214.93 cm^{-1} for absorbed case.

The significant changes in deformation frequencies are depicted in Table 1.

Therefore, from the aforementioned analysis, the favorable chemical bonding interactions of gas molecules on CP monolayer which induces significant changes in their vibration properties can be inferred and the changes in vibrational properties can also be a criterion for gas molecules detection.

TABLE I. The calculated vibrational frequencies (cm^{-1}) for isolated CO, CO_2, NH_3, NO, and NO_2 molecules and these gas molecules absorbed on the surface of CP monolayer (gas+CP monolayer). The diatomic molecules has single frequency and tri-atomic gas molecules has three highest vibrational frequencies presented in this table.

Types	**Vibrational frequencies (cm^{-1})**		
	asymmetric vibration	symmetric vibration	deformation vibration
Isolated CO	2115.97	—	—
CO+CP monolayer	2108.05	—	—
Isolated CO_2	2353.09	1314.47	637.50
CO_2+CP monolayer	2345.81	1313.00	627.03
Isolated NH_3	3515.70	3381.54	1619.64
NH_3+CP monolayer	3512.88	3365.15	1611.47
Isolated NO	1687.10	—	—
NO+CP monolayer	1553.27	—	—
Isolated NO_2	1479.32	1266.29	773.07
NO_2+CP monolayer	1495.33	1214.93	684.80

Here, we have computed the I-V response in x- (armchair direction) and y-direction (zigzag direction) due to their anisotropic nature of electronic properties. The variation of current with applied voltage follows Ohmic law in x-direction while y-direction not follows the Ohmic law. According to linear increment of the current I with voltage in x-direction, we have taken x-direction (zigzag direction) for transport calculations of gas absorption on CP monolayer.

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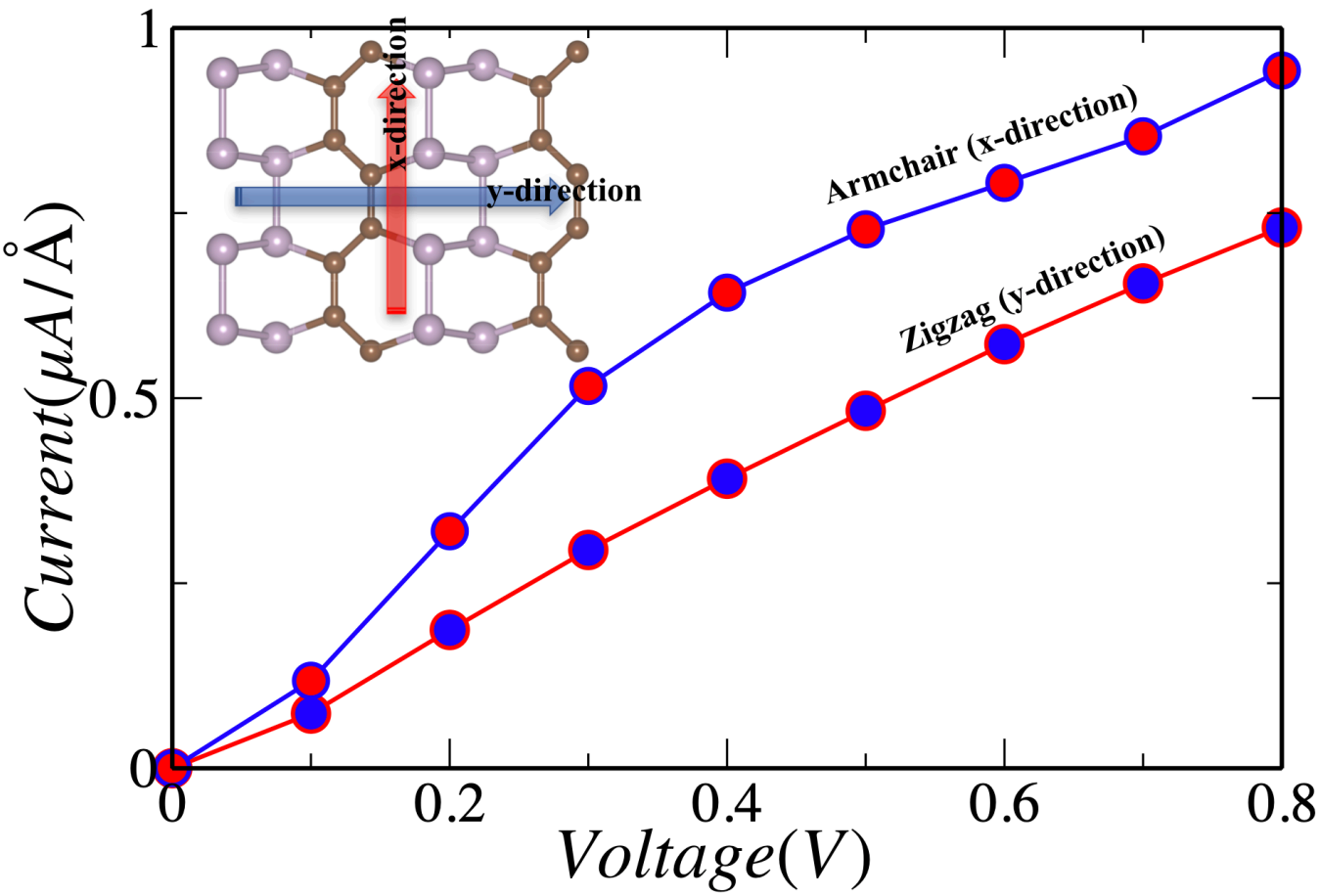

FIG. S1. Anisotropic behaviour of current corresponding applied voltage along the armchair (x-direction) and zigzag (y-direction) directions. Inside the structure shows the armchair and zigzag direction of atomic arrangement. The brown and gray color represents the carbon and phosphorus atoms.