Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

From Fundamental to CO_2 and $COCl_2$ Gas Sensing Properties of Pristine and Defective Si_2BN Monolayer

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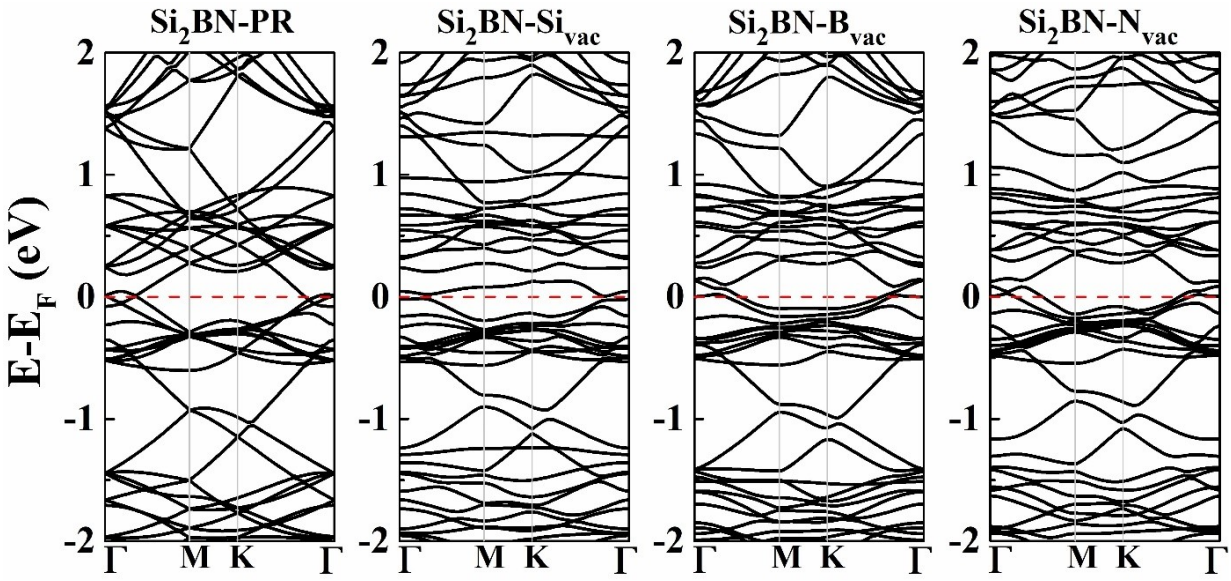

Fig. S1. Calculated electronic band structure of pristine and defective Si_2BN-ML along the Γ-M-K- Γ path using PBE functional showing the metallic characteristics. The horizontal red dashed line represents the Fermi level and is set to 0 eV.

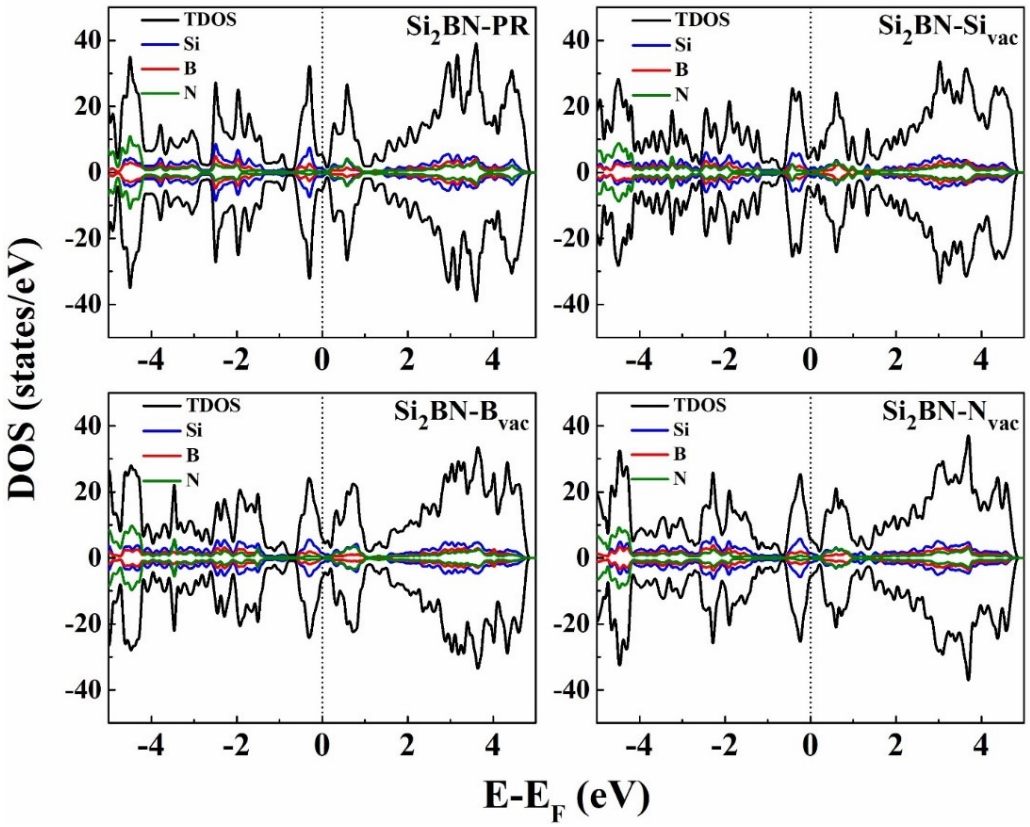

Fig. S2. Computed total and partial electronic densities of states of pristine and defective Si_2BN-ML. The vertical black dashed line represents the Fermi level, which is set to 0 eV.

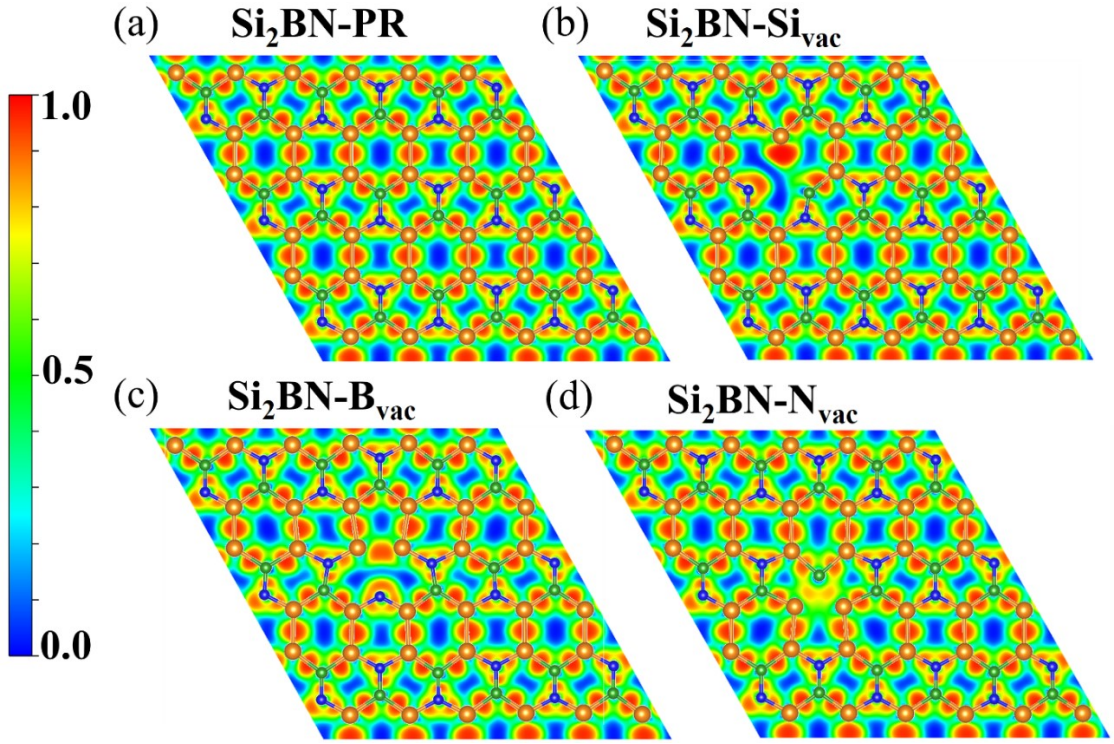

Fig. S3. Electron localization function (ELF) map of pristine and defective Si_2BN-ML with a slice crossing the structure plane. In the ELF maps, the blue and red colors refer to the lowest (0.0) and highest (1.0) value of ELF, indicating depletion and accumulation of electrons at different regions, respectively. The isosurface value for the ELF is 0.508×10^{-3} e/Bohr^3.

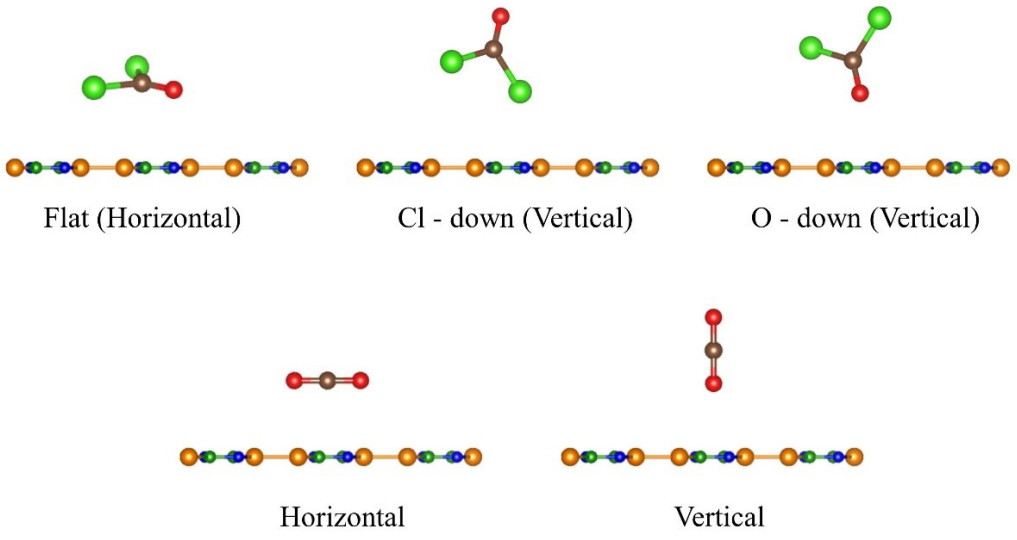

Fig. S4. Possible orientations of $COCl_2$ and CO_2 molecules on the surface of pristine and defective Si_2BN-ML.

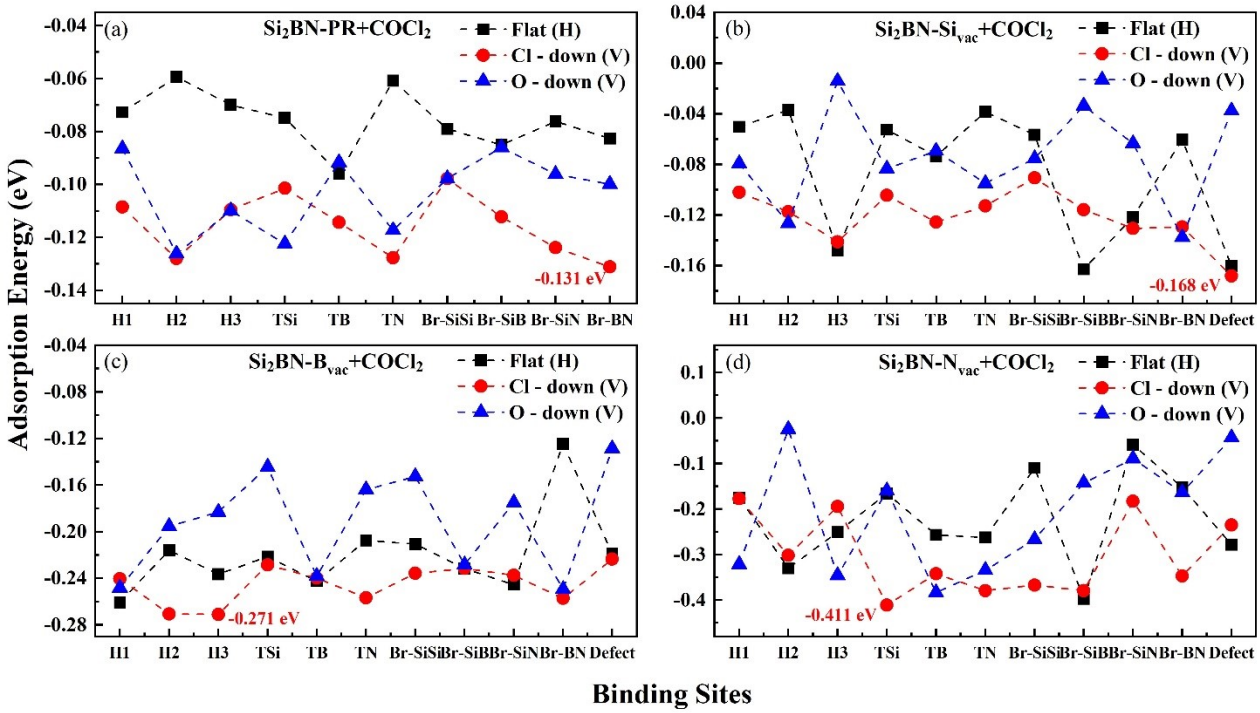

Fig. S5. Computed adsorption energy of $COCl_2$ molecule placed horizontally and vertically on the surface of pristine and defective Si_2BN-ML. The dashed lines are added to guide the eye.

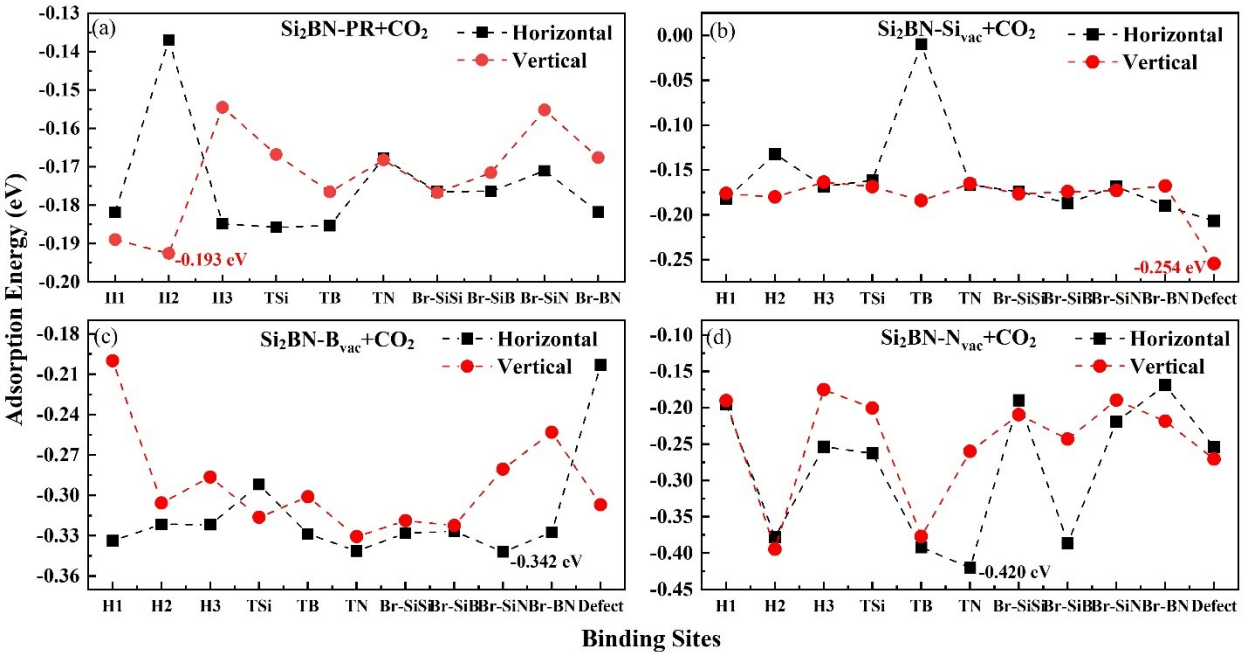

Fig. S6. Computed adsorption energy of CO_2 molecule placed horizontally and vertically on the surface of pristine and defective Si2BN-ML. The dashed lines are added to guide the eye.

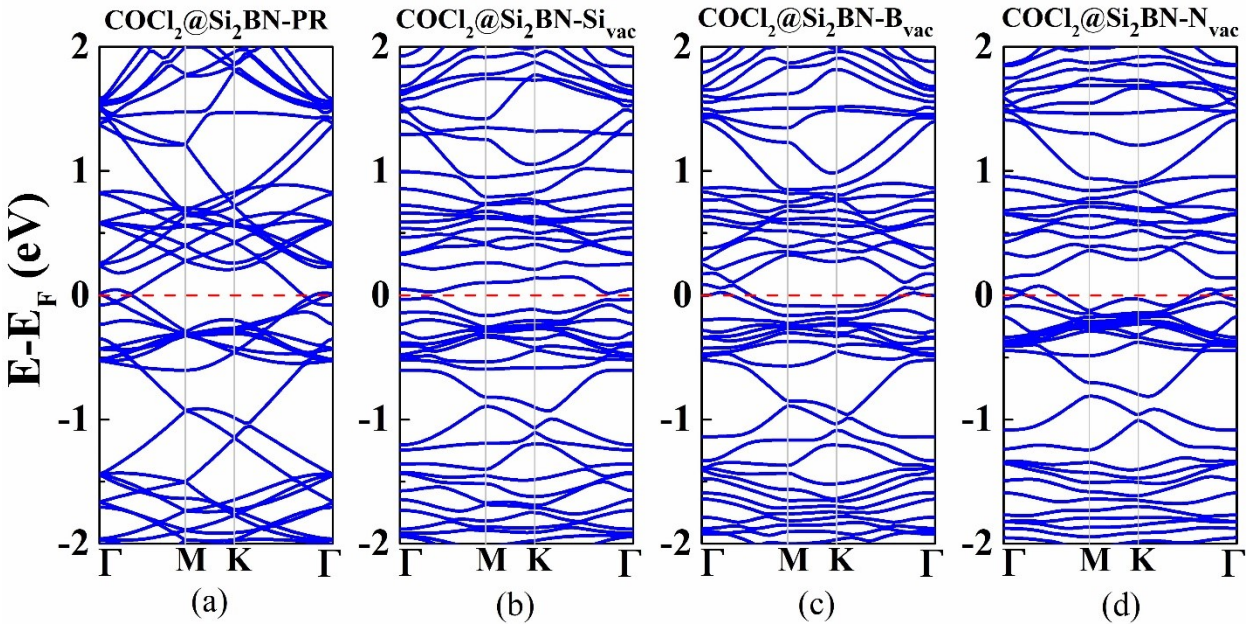

Fig. S7. Calculated electronic band structure when a $COCl_2$ gas molecule adsorbed on pristine and defective Si_2BN-ML obtained using the PBC functional. The horizontal red dashed line represents the Fermi level.

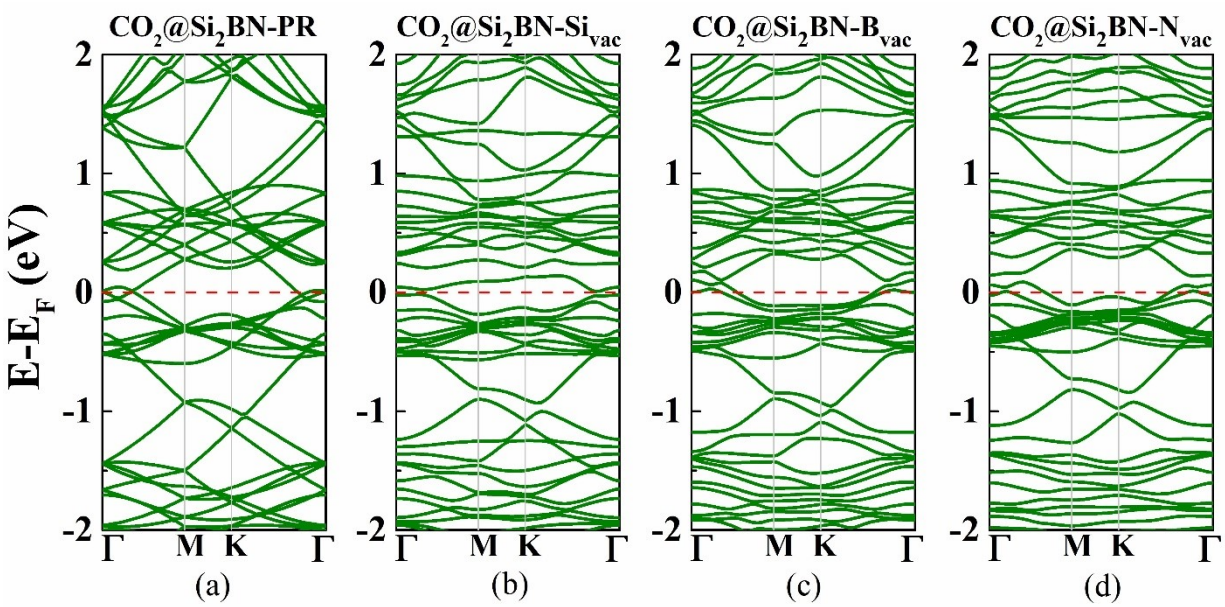

Fig. S8. Calculated electronic band structure when a CO_2 gas molecule adsorbed on pristine and defective Si_2BN-ML obtained using the PBC functional. The horizontal red dashed line represents the Fermi level.

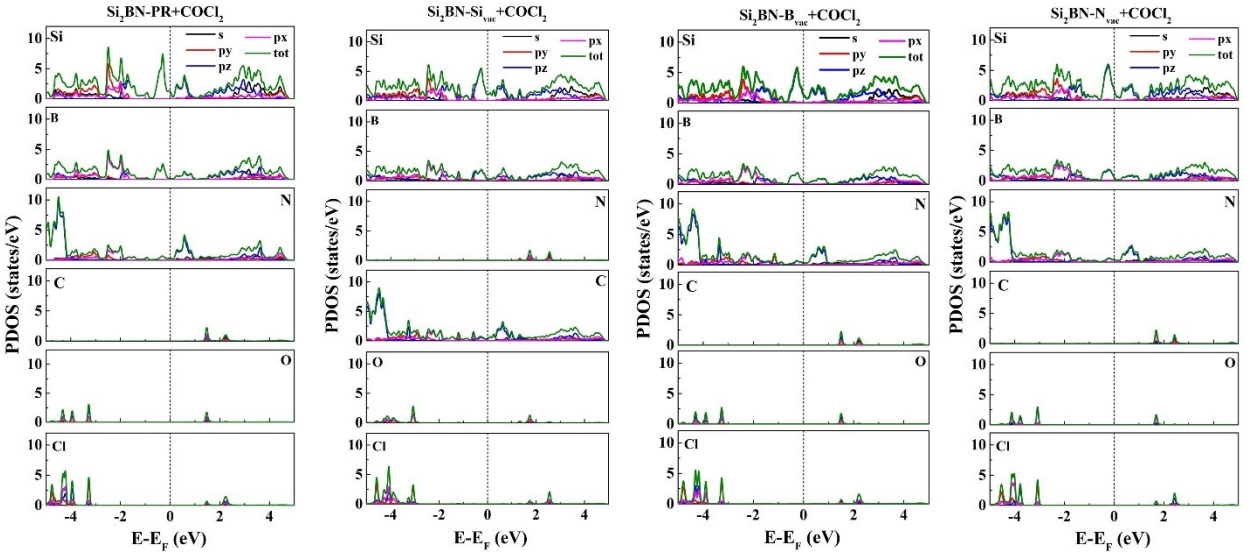

Fig. S9. The projected density of states (PDOS) of $COCl_2$ gas molecule adsorbed on pristine and defective Si_2BN-ML computed using the PBC functional. The vertical black dashed line represents the Fermi level.

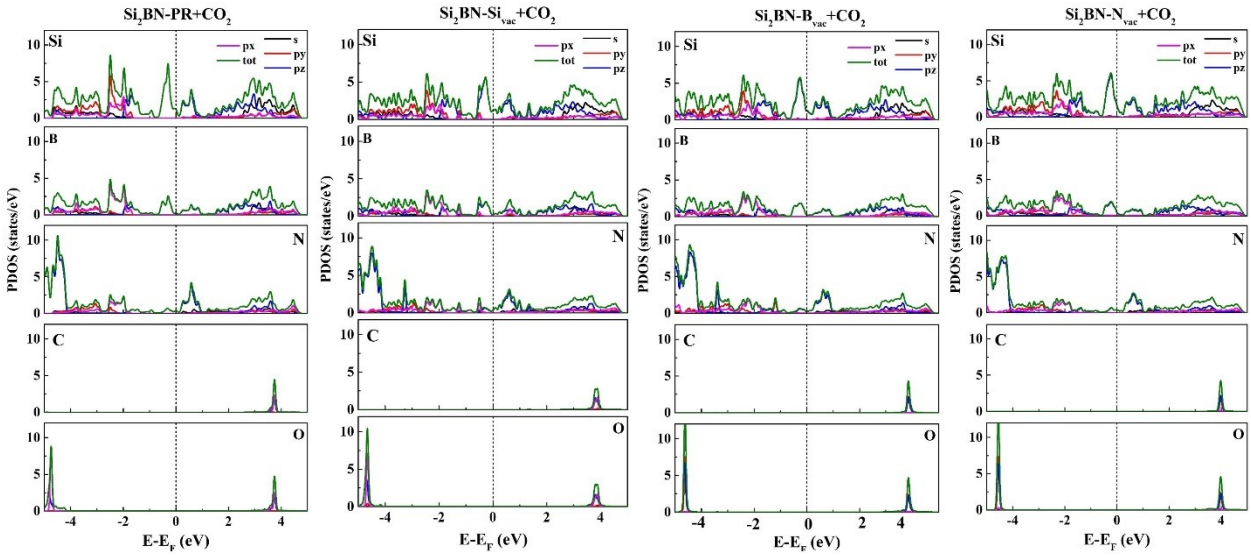

Fig. S10. The projected density of states (PDOS) of CO_2 gas molecule adsorbed on pristine and defective Si_2BN-MLcomputed using the PBC functional. The vertical black dashed line represents the Fermi level.

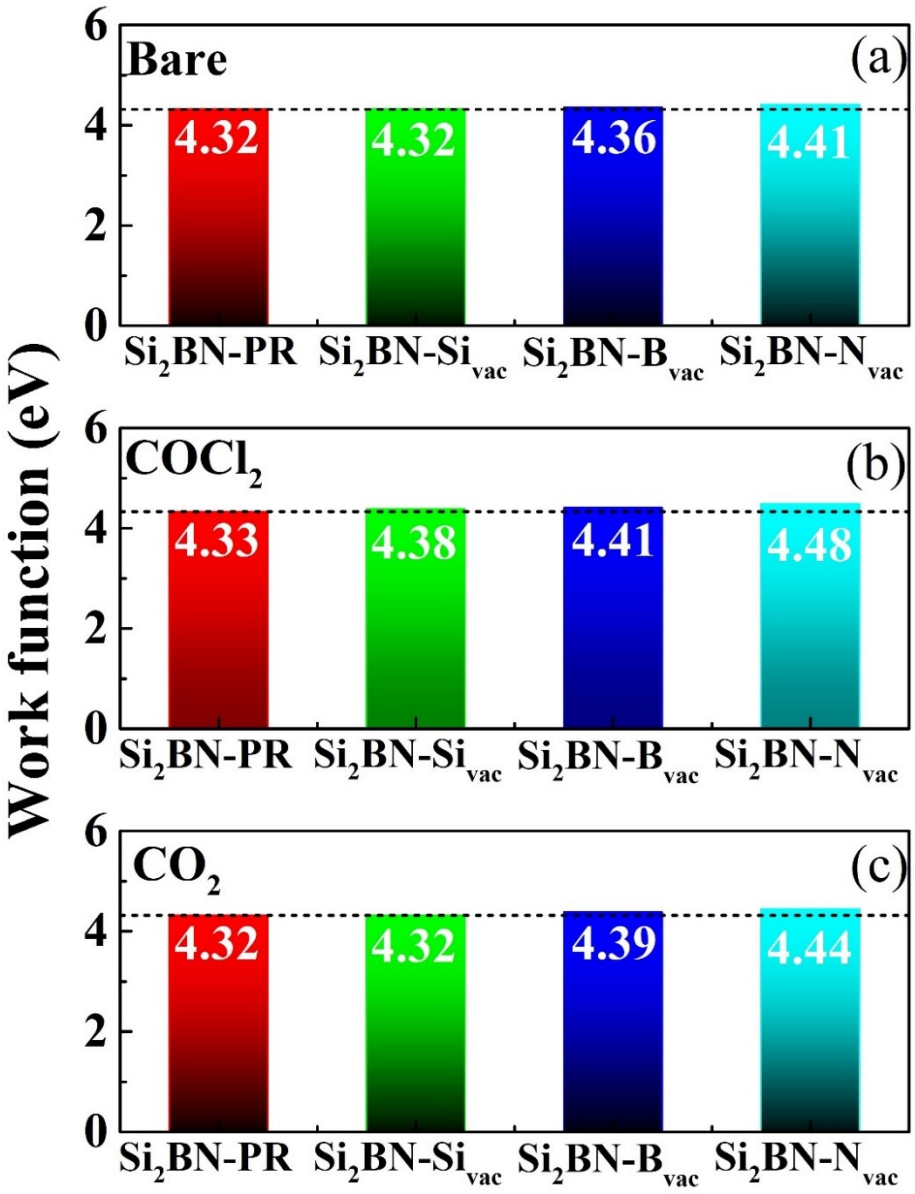

Fig. S11. Computed work function (Φ) of bare, $COCl_2$ and CO_2 gas molecules adsorbed pristine and defective Si_2BN-ML.

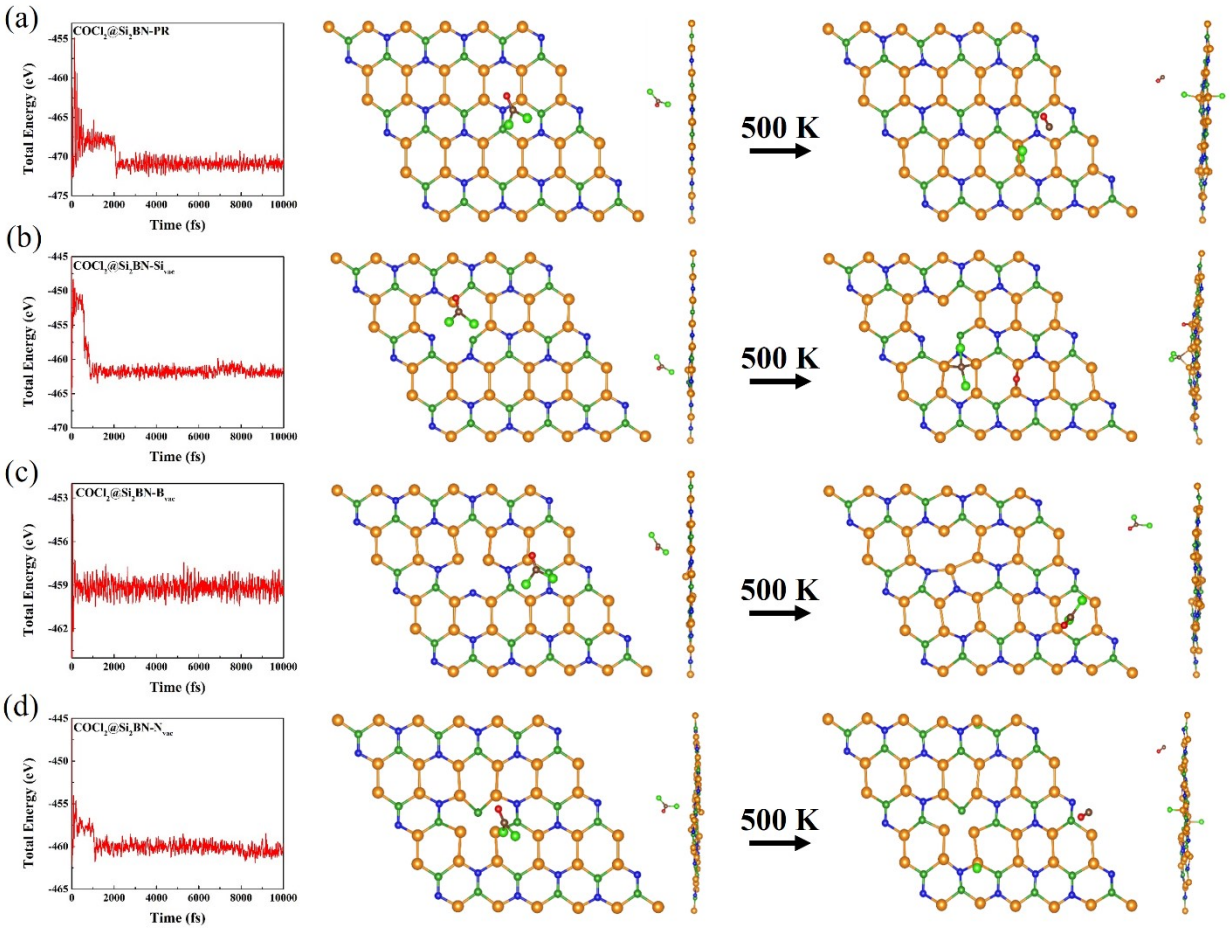

Fig. S12. Fluctuation of total potential energy during the AIMD simulation of $COCl_2$ molecule adsorbed on the surface of (a) Si_2BN-PR, (b) Si_2BN-Si_{vac}, (c) Si_2BN-B_{vac} and (d) Si_2BN-N_{vac} at 500 K. The top and side views of the initial structures, as well as the final structures at the end of the 10 ps AIMD simulation is also provided.

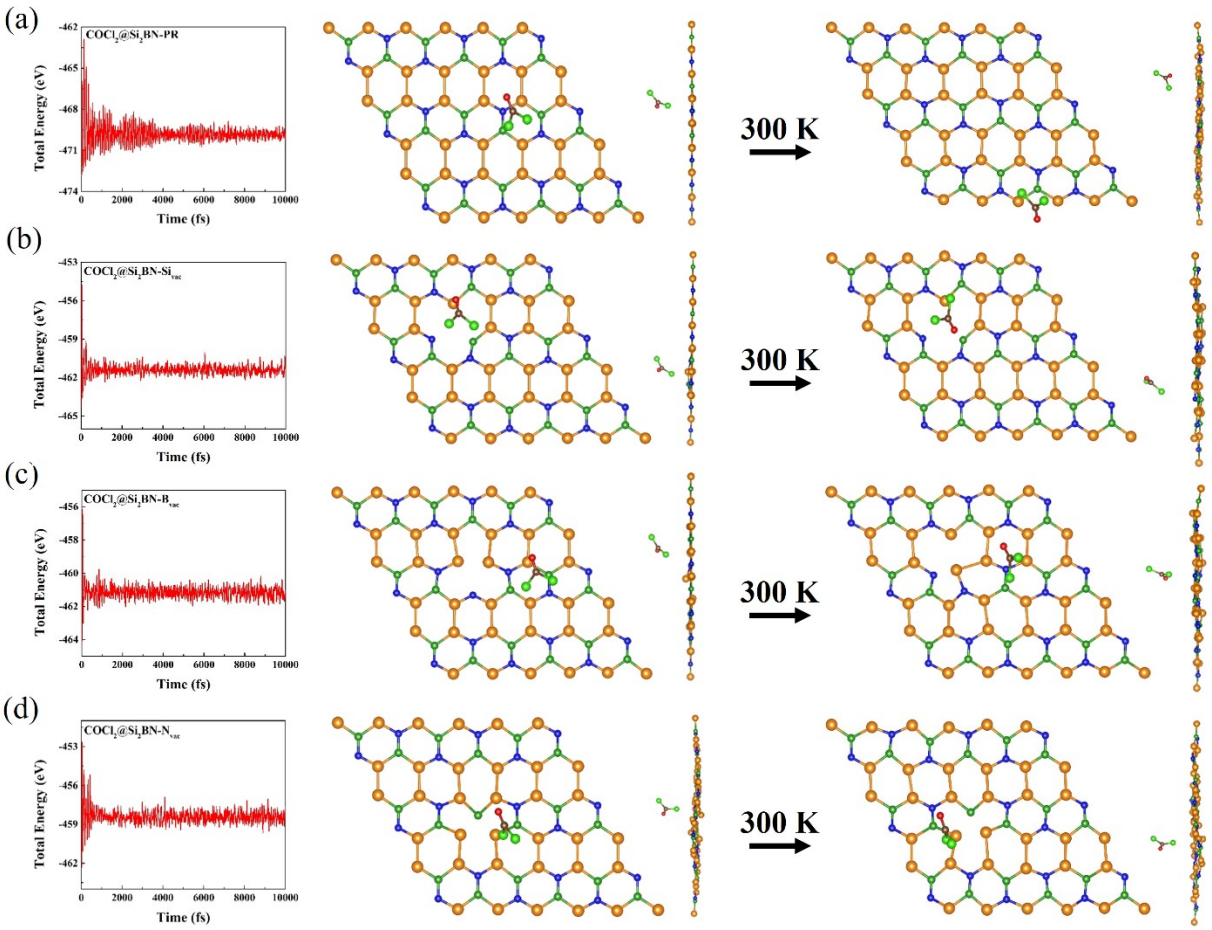

Fig. S13. Fluctuation of total potential energy during the AIMD simulation of $COCl_2$ molecule adsorbed on the surface of (a) Si_2BN-PR, (b) Si_2BN-Si_{vac}, (c) Si_2BN-B_{vac} and (d) Si_2BN-N_{vac} at 300 K. The top and side views of the initial structures, as well as the final structures at the end of the 10 ps AIMD simulation is also provided.

Table S1. The calculated elastic constants, direction-dependent Young's modulus and Poisson's ratio of pristine and defective Si_2BN-ML with the presence of $COCl_2$ and CO_2 molecules.

Molecule	System	Elastic Constants (N/m)				Young's Modulus (N/m)		Poisson's Ratio	
		C_{11}	C_{22}	C_{12}	C_{66}	E_a	E_b	ν_a	ν_b
$COCl_2$	Si_2BN-PR	133	146	43	41	120	134	0.32	0.29
	Si_2BN-Si_{vac}	87	84	14	25	85	82	0.16	0.16
	Si_2BN-B_{vac}	103	113	27	32	96	106	0.26	0.24
	Si_2BN-N_{vac}	81	115	18	32	77	112	0.22	0.16
CO_2	Si_2BN-PR	134	145	42	41	120	133	0.32	0.29
	Si_2BN-Si_{vac}	103	107	35	24	91	96	0.34	0.33
	Si_2BN-B_{vac}	86	122	31	24	75	114	0.36	0.25
	Si_2BN-N_{vac}	118	114	31	36	109	106	0.26	0.27