Potential of nanostructured carbon materials for iodine detection in realistic environments revealed by first-principles calculations: Supporting information

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Figures S1 to S4 depict different trial initial geometries of molecules placed over different substrates, arbitrarily labelled throughout (a, b, etc.) within each pair (molecule + substrate).

Table S1 lists adsorption energies in final (relaxed) configurations, stemming from the numbered start configurations of Figs S1–S4.

Table S2 specifies bond lengths in free and adsorbed molecules.

Figures S5 to S8 depict partial densities of states for atoms involved in the adsorption of four trial molecules on C_3N monolayer.

Table S3 characterises charge transfer (specified within the Bader analysis) between four trial molecules and the C_3N substrate.

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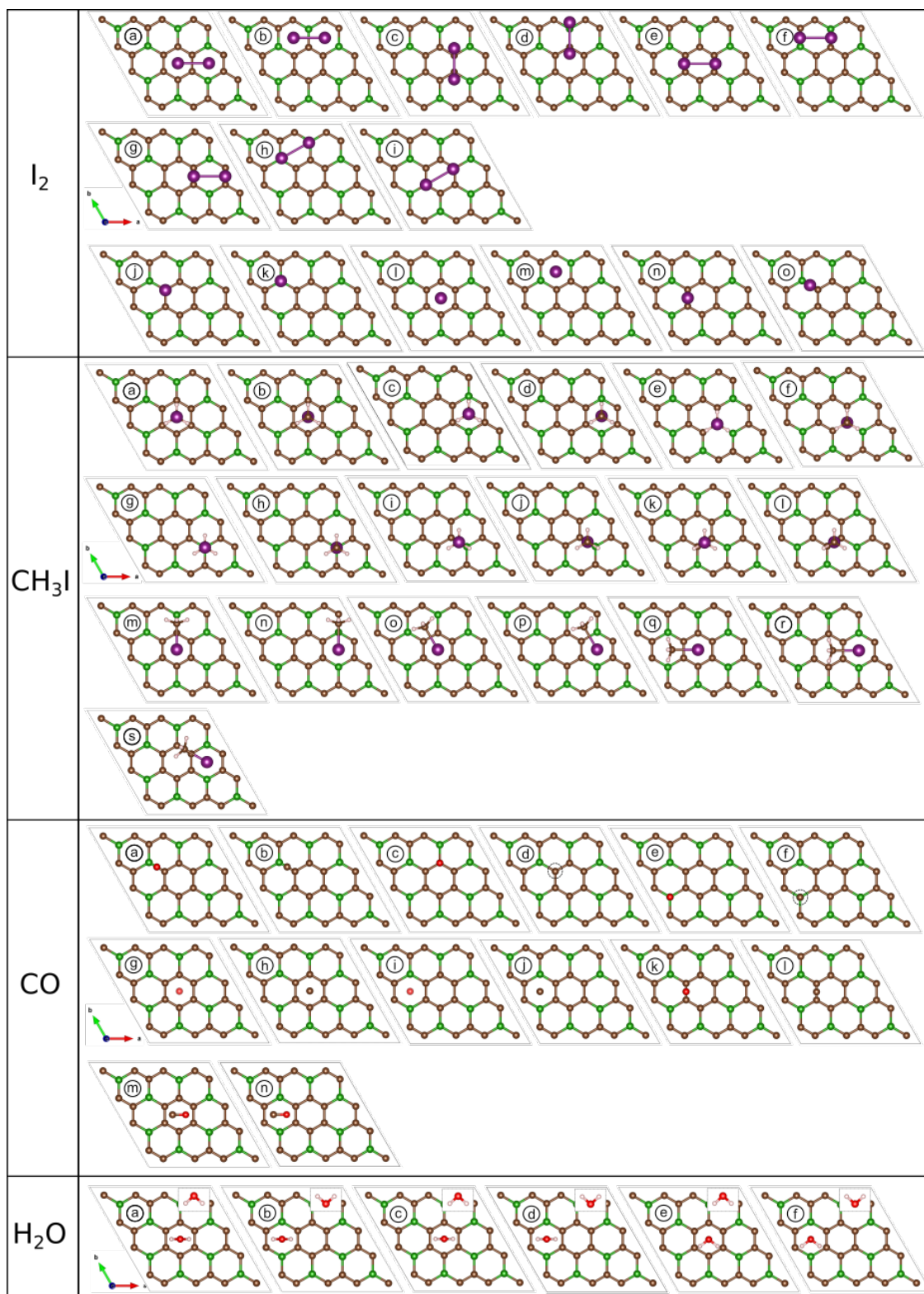[1]Present address: Institut für Physikalische Chemie, Universität Münster, Germany

Figure S1: Top and side views of the considered adsoption position of I_2, CH_3I, CO, and H_2O molecules on BC_3 sheet.
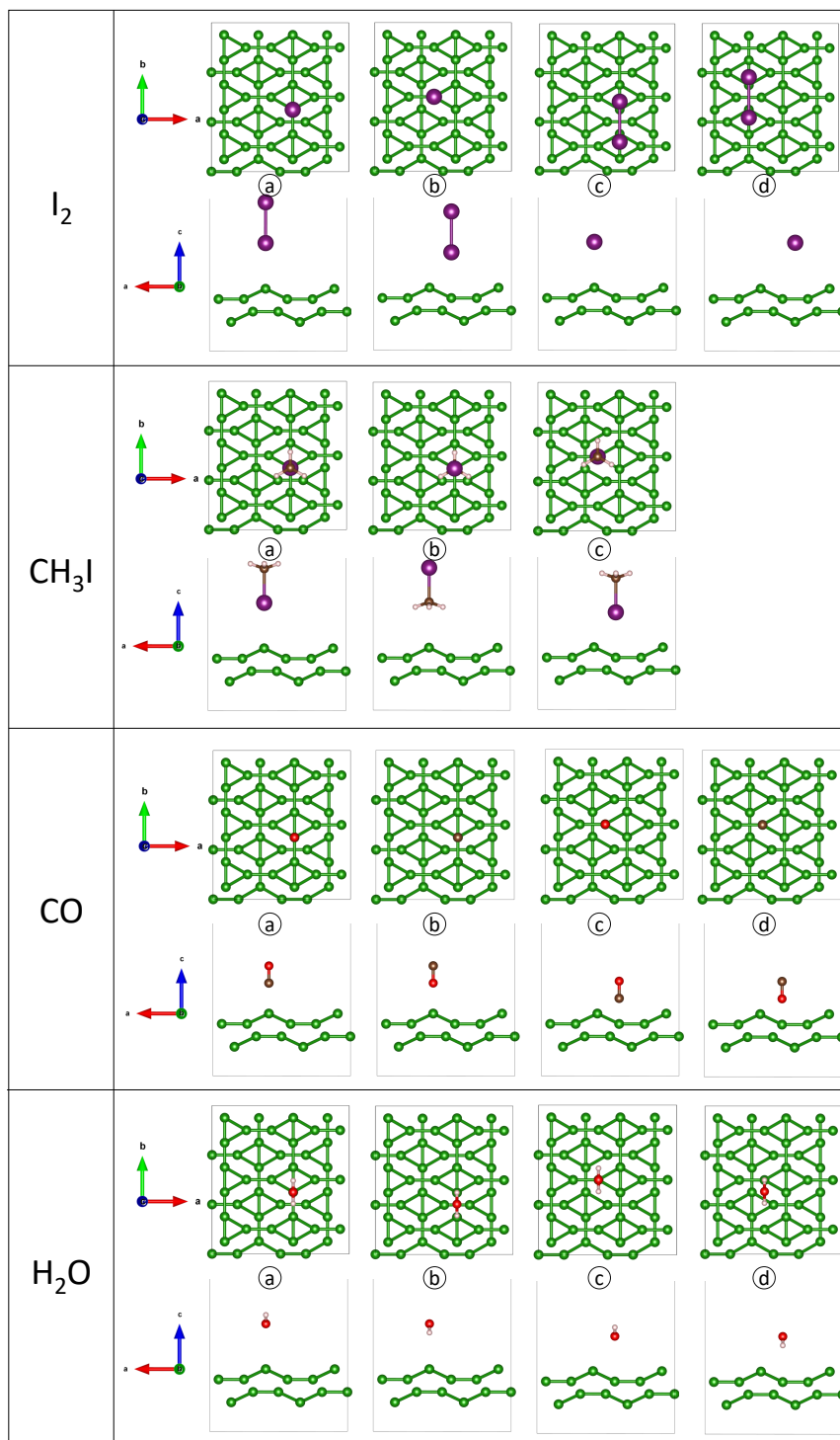
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Figure S2: Top and side views of the considered adsoption position of I_2, CH_3I, CO, and H_2O molecules on 8-$Pmmn$ borophene.
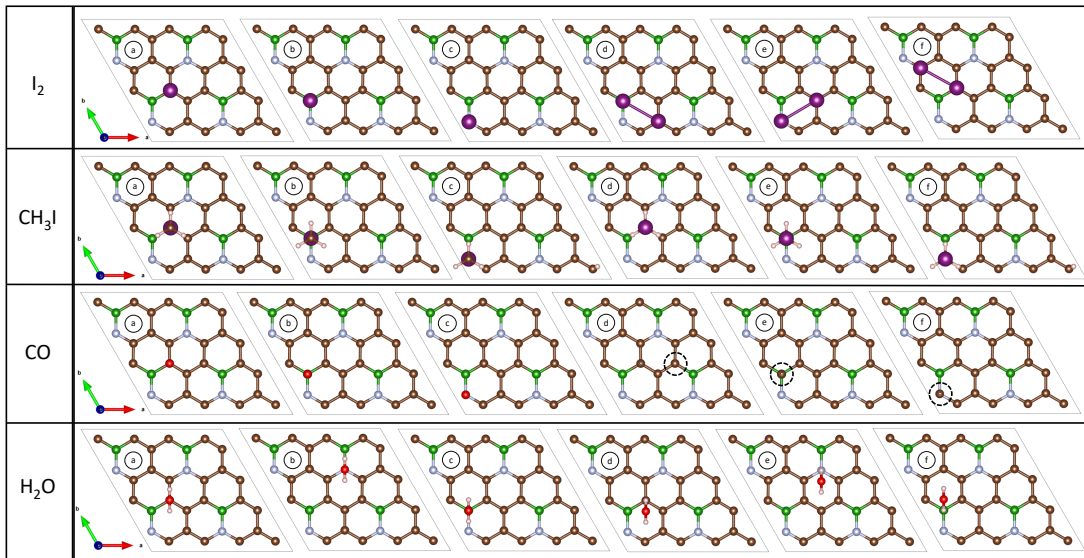
Figure S3: Top and side views of the considered adsoption position of I_2, CH_3I, CO, and H_2O molecules on BC_6N-2 sheet.
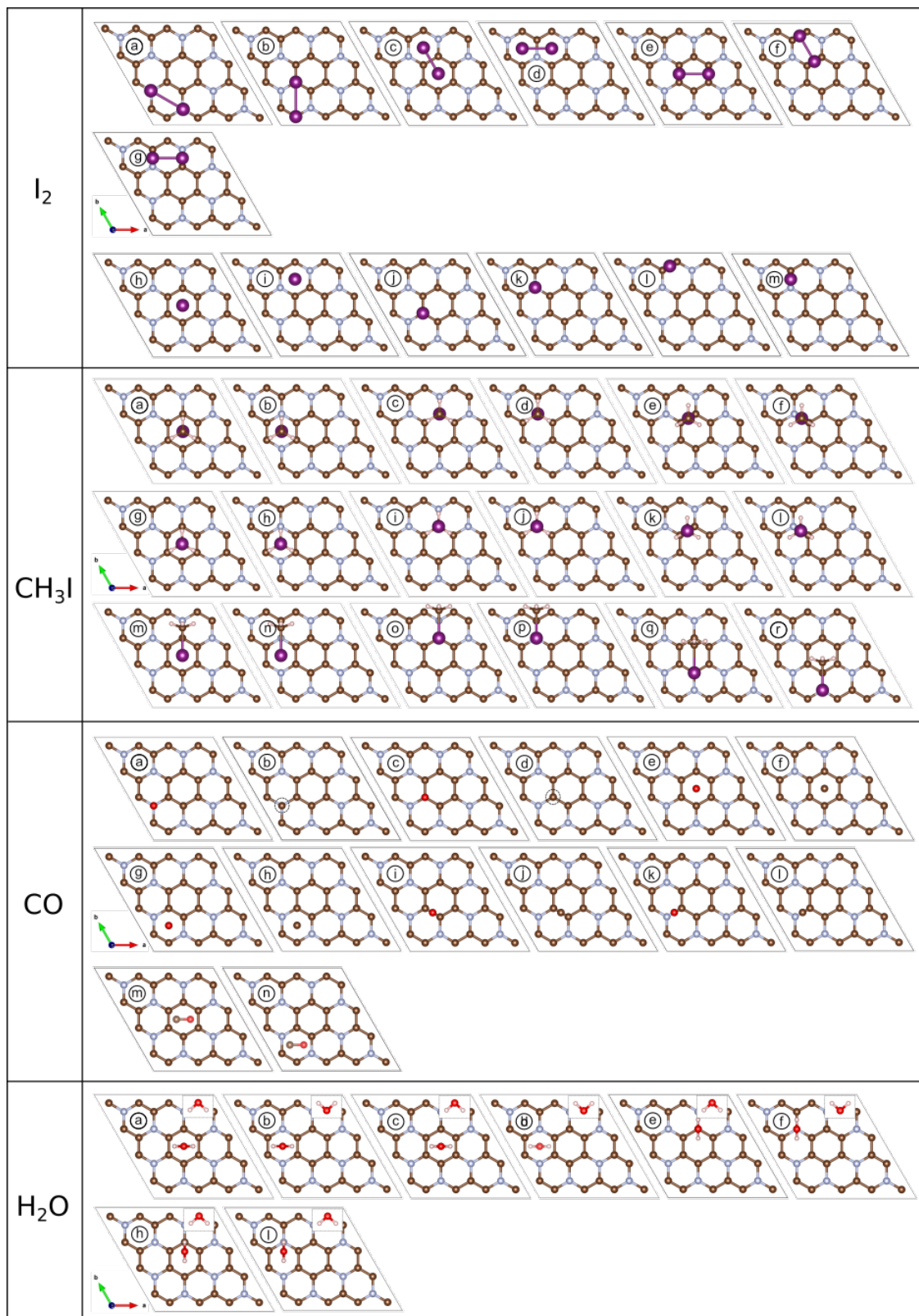
Figure S4: Top and side views of the considered adsoption position of I_2, CH_3I, CO, and H_2O molecules on C_3N sheets.

Table S1: Adsorption energies in eV of I_2, CH_3I, CO, and H_2O molecules for different sites on BC_3, 8-*Pmmn* borophene, BC_6N-2, and C_3N sheets. The corresponding adsorption sites are shown in Fig. S1–S4. The largest adsorption energy for each (molecule / substrate) pair is indicated in boldface.

Site	BC₃				8-*Pmmn* borophene				BC₆N-2				C₃N			
	I_2	CH_3I	CO	H_2O	I_2	CH_3I	CO	H_2O	I_2	CH_3I	CO	H_2O	I_2	CH_3I	CO	H_2O
a	−0.35	−0.15	−0.75	−0.15	**−0.66**	−0.29	−0.55	−0.14	**−0.40**	**−0.27**	**−0.12**	−0.07	−0.80	−0.28	−0.10	−0.17
b	−0.33	−0.21	−0.08	−0.21	−0.48	−0.18	−0.06	−0.12	−0.39	−0.26	−0.12	−0.15	−0.75	−0.25	−0.08	**−0.19**
c	**−0.49**	−0.19	−0.11	−0.06	−0.38	**−0.35**	**−0.65**	−0.17	−0.39	−0.23	−0.11	−0.15	−0.78	−0.28	−0.12	−0.07
d	−0.38	−0.27	−0.09	−0.12	−0.54	—	−0.12	**−0.24**	−0.33	−0.19	−0.11	−0.17	**−0.80**	−0.24	−0.07	−0.12
e	−0.29	−0.18	**−0.75**	−0.15	—	—	—	—	−0.33	−0.21	−0.08	**0.17**	−0.76	−0.28	−0.10	−0.18
f	−0.49	−0.26	−0.07	**−0.21**	—	—	—	−0.12	−0.35	−0.20	−0.08	−0.14	−0.73	−0.28	−0.07	−0.10
g	−0.28	−0.19	−0.07	—	—	—	—	—	—	—	—	—	−0.80	−0.18	−0.10	−0.19
h	−0.49	−0.21	−0.06	—	—	—	—	—	—	—	—	—	−0.56	−0.21	−0.09	−0.13
i	−0.28	−0.19	−0.07	—	—	—	—	—	—	—	—	—	−0.55	−0.20	−0.13	—
j	−0.44	−0.27	−0.06	—	—	—	—	—	—	—	—	—	−0.60	−0.22	−0.15	—
k	−0.27	−0.18	−0.09	—	—	—	—	—	—	—	—	—	−0.51	−0.21	−0.11	—
l	−0.26	−0.26	−0.06	—	—	—	—	—	—	—	—	—	−0.60	−0.22	−0.08	—
m	−0.37	−0.28	−0.10	—	—	—	—	—	—	—	—	—	−0.60	−0.33	**−0.15**	—
n	−0.42	**−0.44**	−0.08	—	—	—	—	—	—	—	—	—	—	−0.33	−0.13	—
o	−0.43	−0.28	—	—	—	—	—	—	—	—	—	—	—	**−0.34**	—	—
p	—	−0.31	—	—	—	—	—	—	—	—	—	—	—	−0.32	—	—
q	—	−0.28	—	—	—	—	—	—	—	—	—	—	—	−0.31	—	—
r	—	−0.35	—	—	—	—	—	—	—	—	—	—	—	−0.32	—	—
s	—	−0.40	—	—	—	—	—	—	—	—	—	—	—	—	—	—

Table S2: Selected bond lengths (in Å) in free and adsorbed molecules. The absolute change of the bond length relative to free molecule is shown in parentheses.

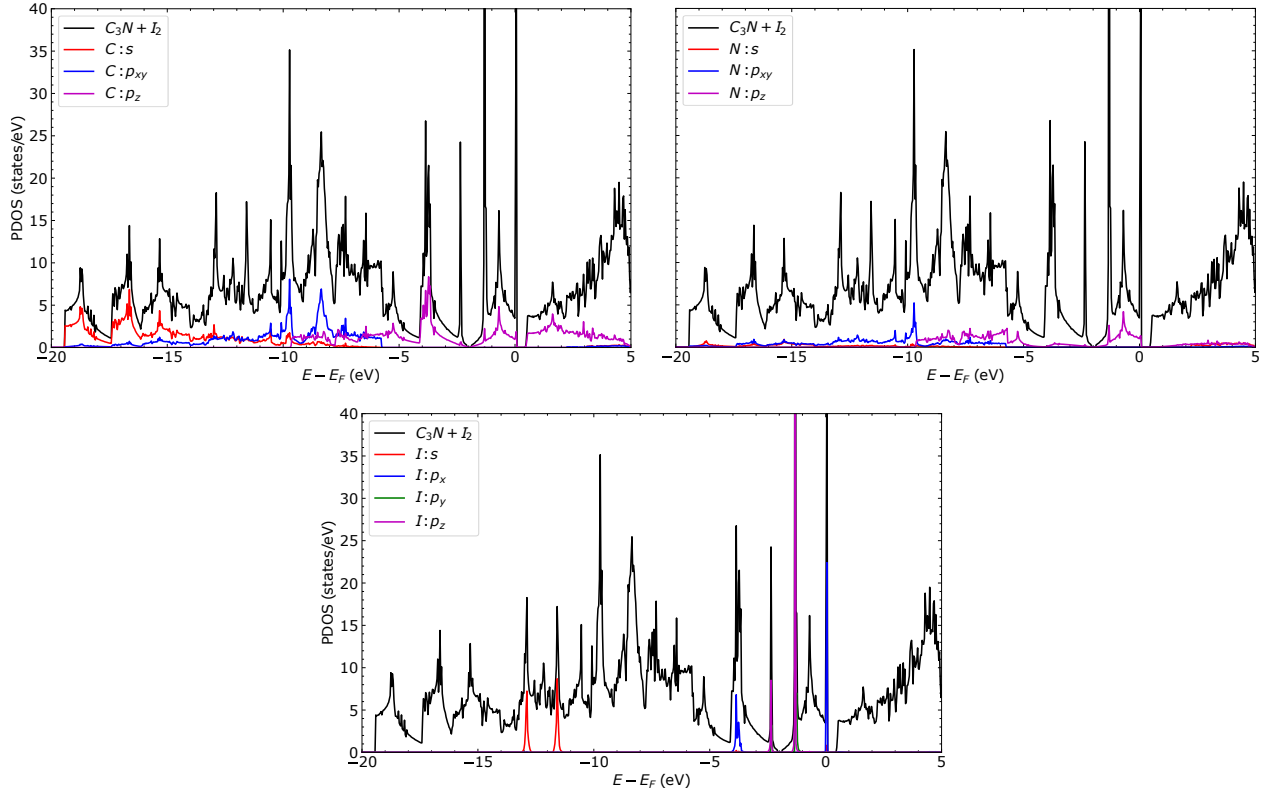| Molecule:	I_2	CH_3I		CO	H_2O
Bond:	I–I	C–I	C–H	C–O	H–O
In free molecule:	2.68	2.16	1.09	1.14	0.97
On BC_3:	2.67 (−0.01)	2.15 (0.01)	1.09 (0.00)	1.15 (0.01)	0.97 (0.00)
On 8-$Pmmn$ borophene:	2.72 (0.04)	2.16 (0.00)	1.09 (0.00)	1.14 (0.00)	0.97 (0.00)
On BC_6N-2:	2.82 (0.13)	2.16 (0.00)	1.09 (0.00)	1.15 (0.01)	0.97 (0.00)
On C_3N:	2.92 (0.24)	2.16 (0.00)	1.09 (0.00)	1.14 (0.00)	0.97 (0.00)

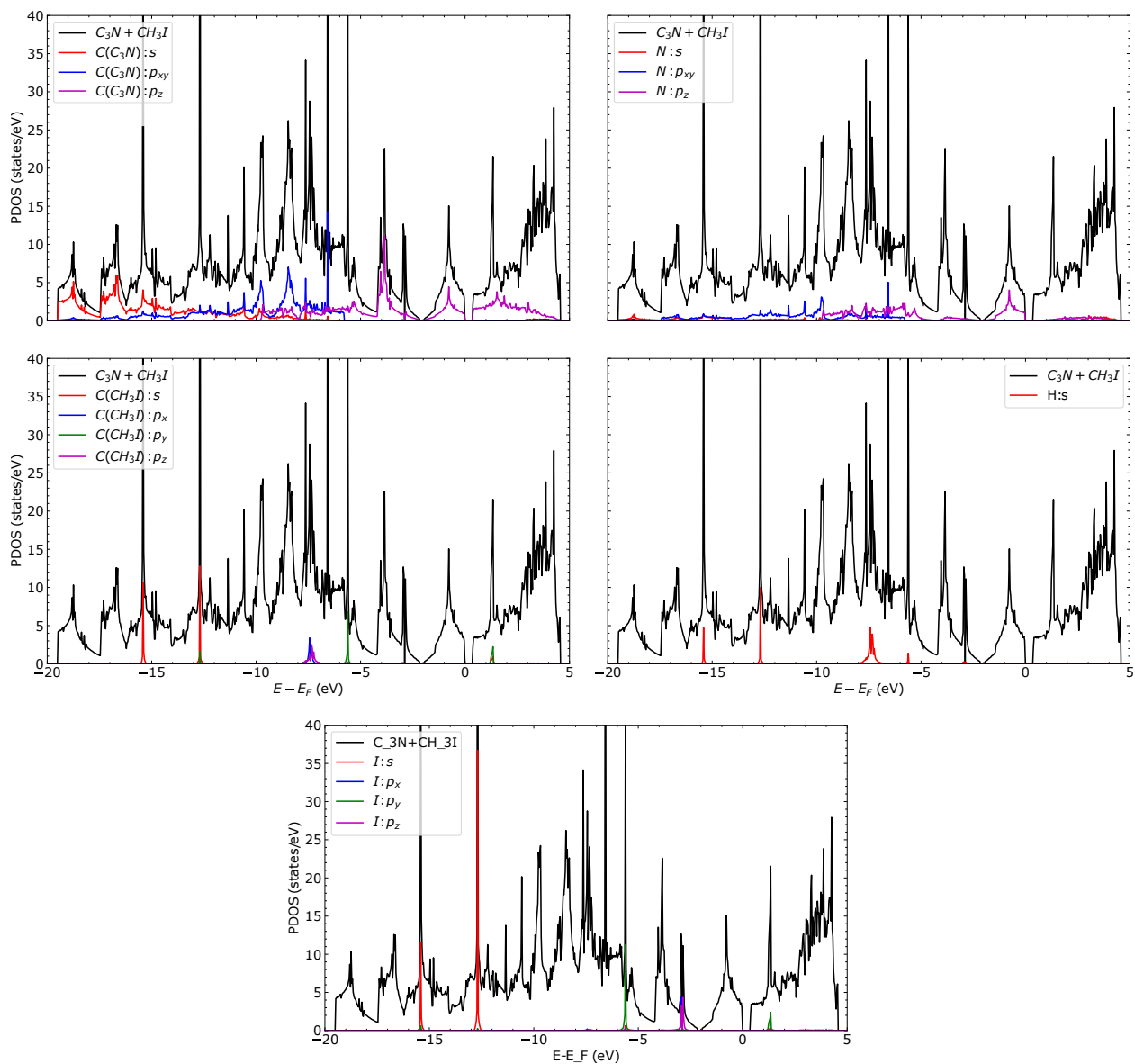Figure S5: Partial densities of states for atoms concerned by absorption of I_2 on a C_3N sheet.

Figure S6: Partial densities of states for atoms concerned by absorption of CH$_3$I on a C$_3$N sheet.

Table S3: Charge transfer (in e, derived from the Bader analysis) accompanying the relaxed configuration with the strongest adsorption energy of different molecules on C$_3$N. Negative values mean transfer of electrons from the molecule to the substrate.

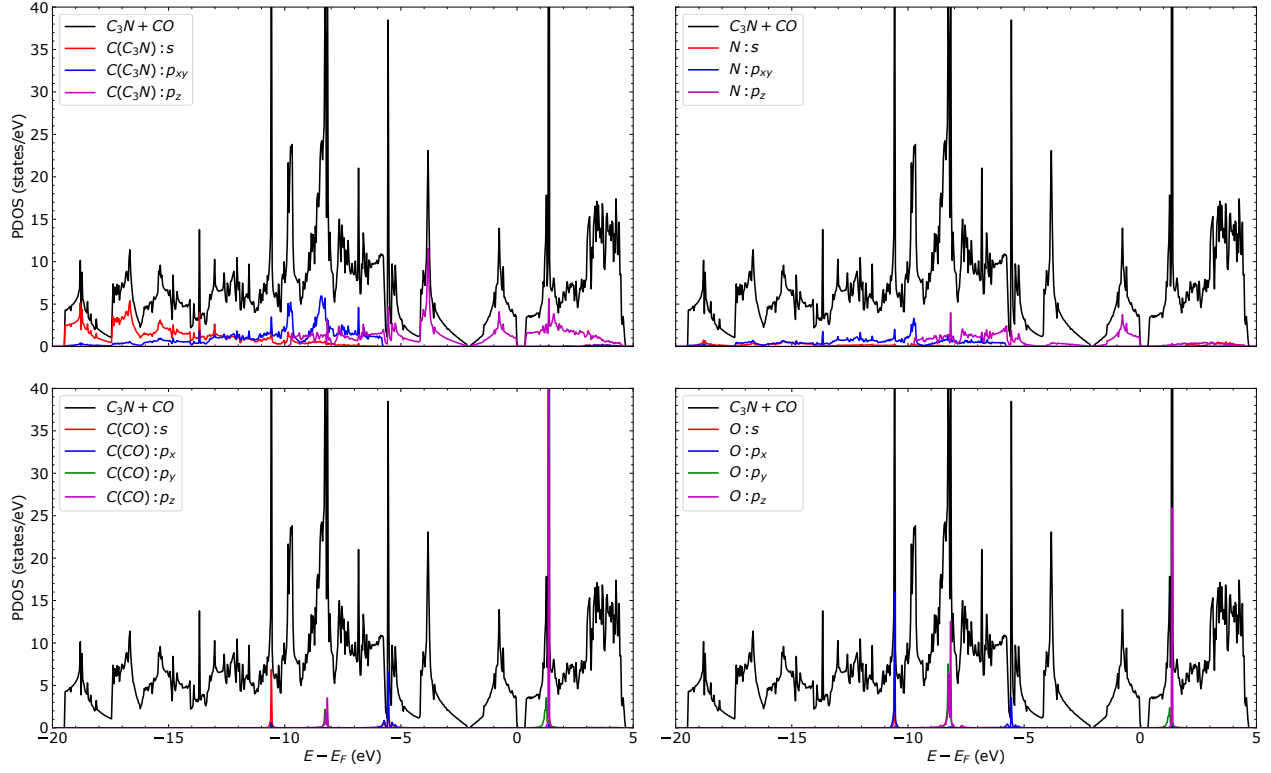| Molecules:	I$_2$	CH$_3$I	CO	H$_2$O
Charge transfer:	-0.43	-0.00	-0.04	-0.02

Figure S7: Partial densities of states for atoms concerned by absorption of CO on a C$_3$N sheet.
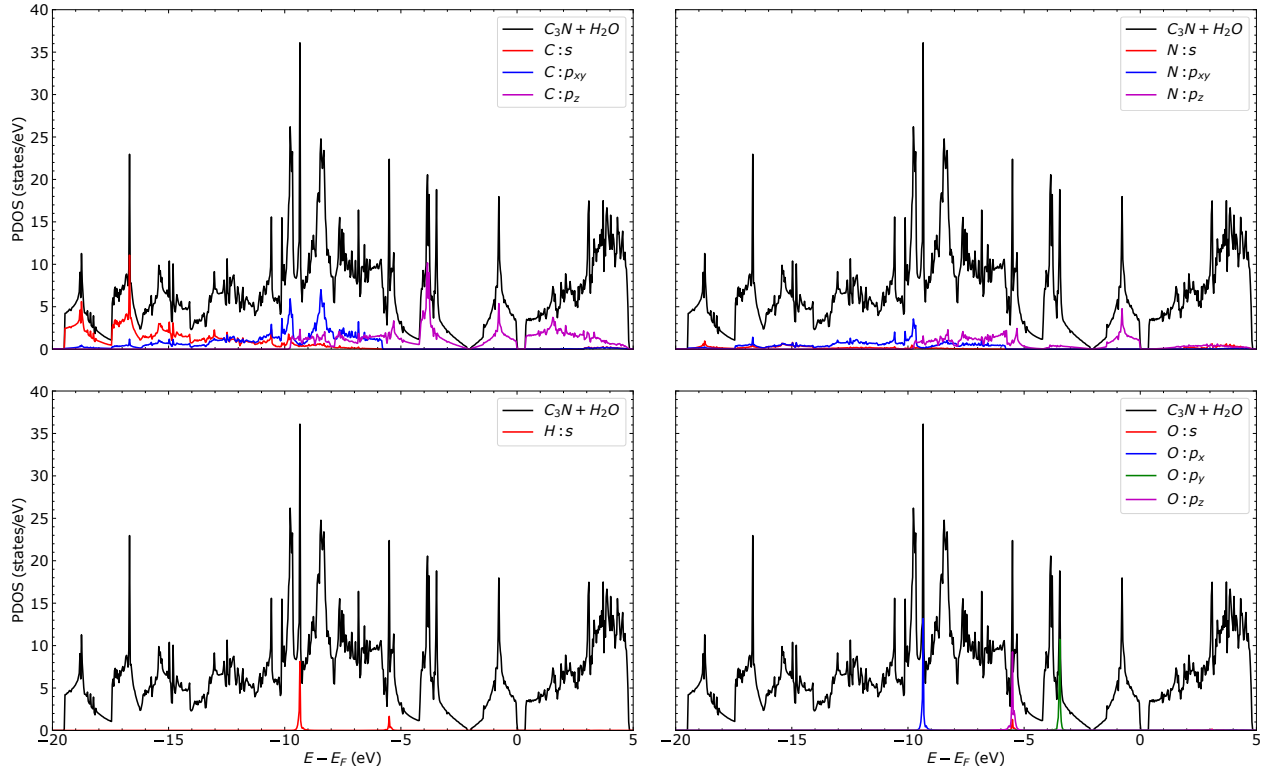

Figure S8: Partial densities of states for atoms concerned by absorption of H$_2$O on C$_3$N sheet.