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Supplementary Information for

The first-principles study of adsorption of the NH_3, NO, and NO_2 gas molecules on InSe-like phosphorus carbide

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Tab. S1
Figs. S1 to S5

The calculated adsorption energy E_a of NH_3, NO, and NO_2 on *γ*-PC, the charge transfer Δq between the adsorbed molecules and the *γ*-PC surface, the shortest distance *d* from the adsorbed molecules to the *γ*-PC surface and the workfunction WF of molecule-adsorbed *γ*-PC for the configurations shown in Figures S1-3 are collected in Table S1.

Table S1. The adsorption energy E_a of different configurations of NH_3, NO, and NO_2 on *γ*-PC; the charge transfer Δq between the adsorbed molecules and the *γ*-PC surface; the shortest distance *d* from the adsorbed molecules to the *γ*-PC surface; the workfunction WF of molecule-adsorbed *γ*-PC.

Molecule	E_a, eV	Role	Δq, *e*	*d*, Å	WF, eV
NH_3	-0.14	donor	-0.003	3.09	5.54
	-0.14	donor	-0.002	3.10	5.50
NO	-0.11	acceptor	0.002	3.11	4.70
	-0.16	donor	-0.009	3.21	4.61
NO_2	-0.50	acceptor	1.072	2.91	5.63
	-0.49	acceptor	1.048	3.07	5.62

The increased charge transfer from the *γ*-PC surface to NO_2 can be attributed to the configuration of the molecule. The electronegativity of oxygen atoms is higher than that of nitrogen atoms, in turn, the electronegativity of nitrogen atoms is higher than that of carbon atoms, while the electronegativity of carbon atoms is higher than that of phosphorus atoms. Therefore, the closer the O atom/atoms to the phosphorus atoms at the surface the higher charge transfer (Tables 1 and S1 and Figure S4).

To show the specific difference between the sensitivity of *γ*-PC to NO and NO_2, the electronic localization function (ELF) of NO and NO_2 molecule-adsorbed *γ*-PC is calculated (Figure S5 a and b). The value of the ELF (between 0 and 1) reflects the degree of the charge localization in the real space, where 0 represents a free electronic state, while 1 represents a perfect localization. The isosurface value of 0.65 is adopted in Figure S5. In both cases, a significant number of electrons are distributed between carbon-carbon and carbon-phosphorus bonds, indicating a strong covalent bonding between carbon atoms and carbon and phosphorus atoms. In addition, a strong charge localization is observed on phosphorus atoms. In the case of NO, a strong depletion of electrons at the oxygen atom of the molecule, a small depletion of electrons at the phosphorus atoms of the surface and a strong electron accumulation at the nitrogen atom of the molecule are observed (Figure S5 a). Clearly, a strong charge transfer redistribution occurs within the NO molecule (this is also confirmed by the Bader analysis), while only a small amount of the charge transfers between the molecule and the surface (mostly from oxygen atoms to phosphorus atoms). Importantly, in the case of NO_2, there is a strong charge transfer from the nearest to the molecule phosphorus atom to the molecule. The charge mostly accumulates at the nitrogen atom by transferring through and from the oxygen atoms (Figure S5 b), which is also confirmed by the Bader analysis. Therefore, based on the results presented in Tables 1 and S1 and the ELF analysis it can be concluded that for NO the configuration of the molecule on *γ*-PC plays a crucial role in its charge transfer ability.

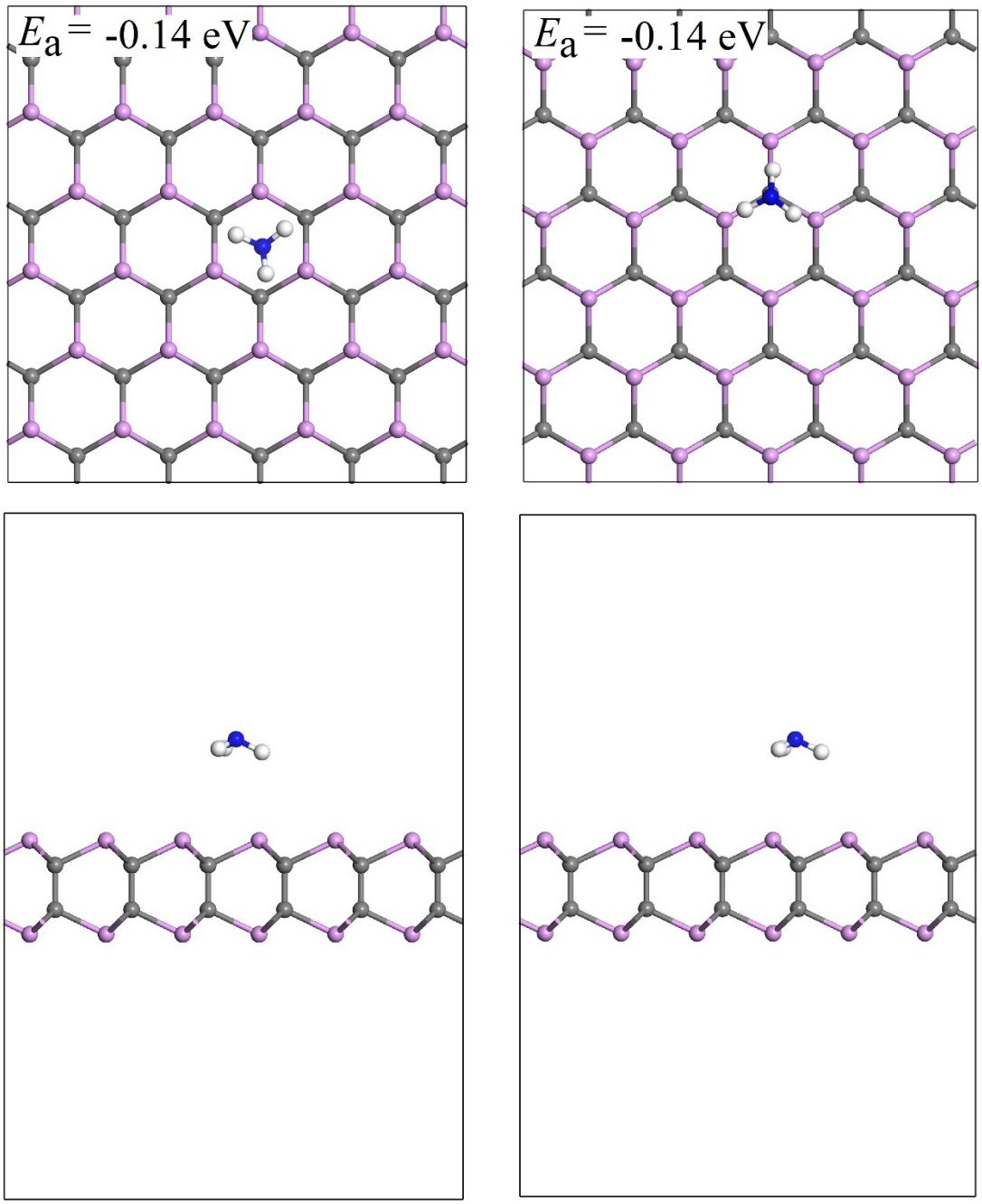

Figure S1. The top and side views of the examined possible absorption configurations of the NH_3 molecule adsorbed on γ-PC.

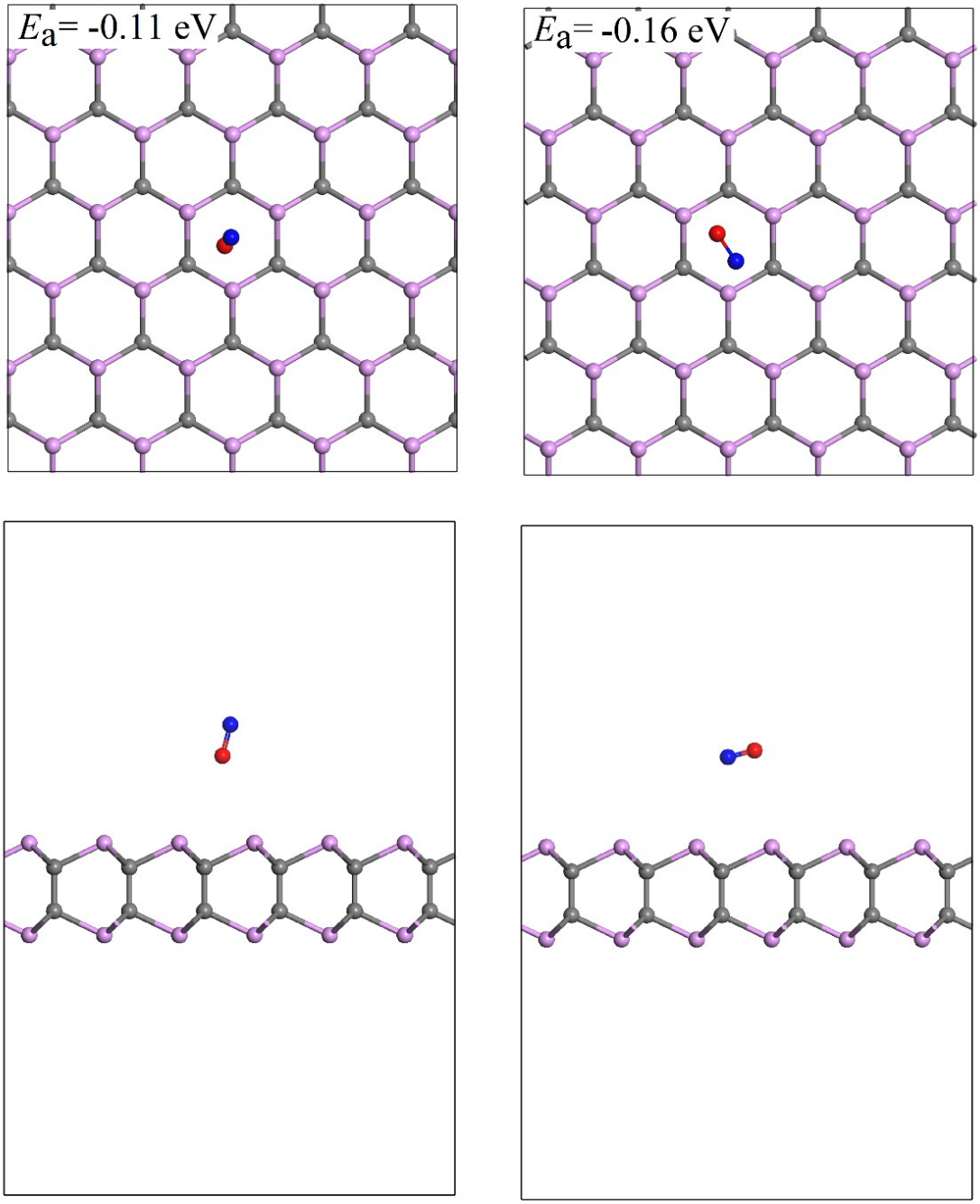

Figure S2. The top and side views of the examined possible absorption configurations of the NO molecule adsorbed on γ-PC.

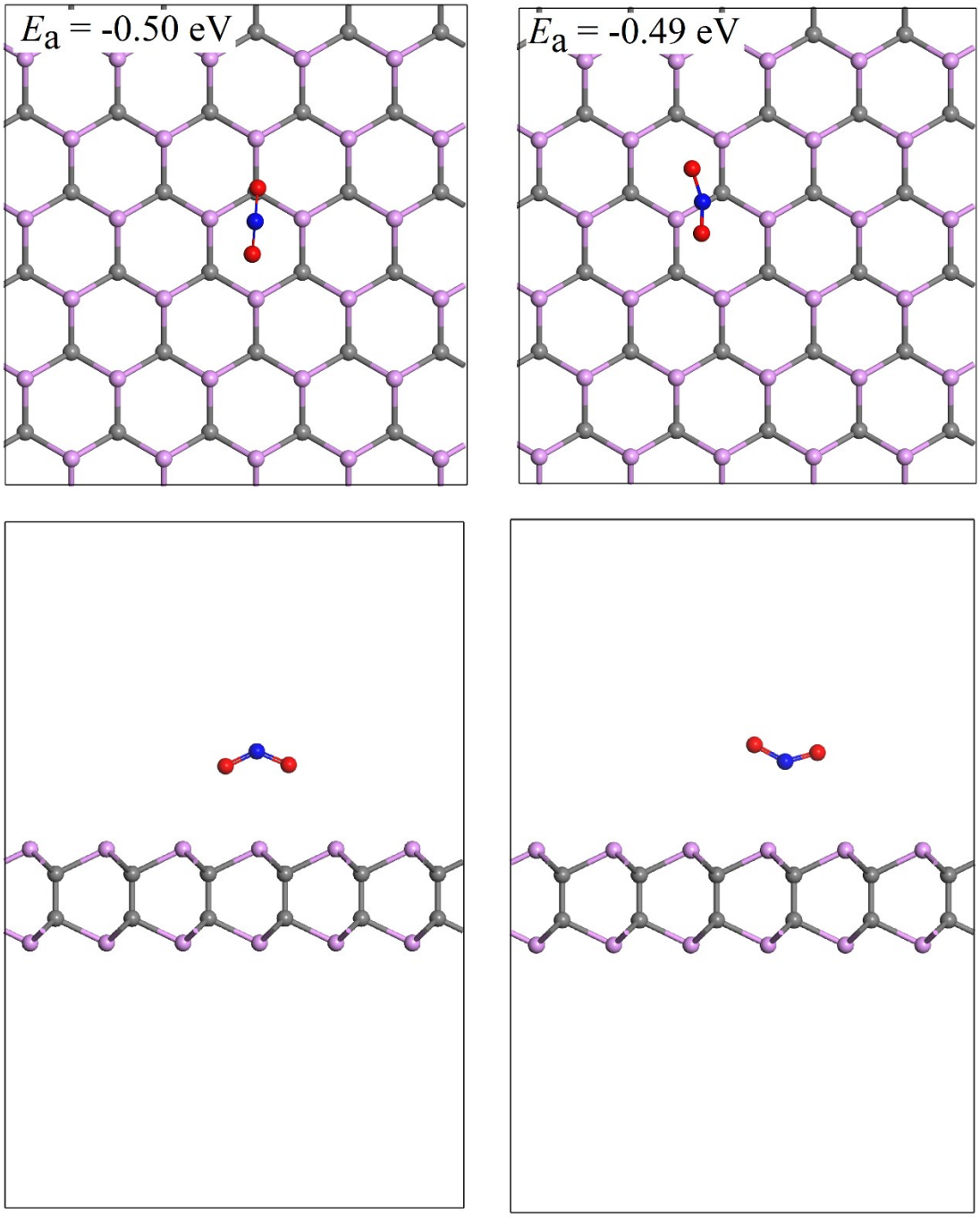

Figure S3. The top and side views of the examined possible absorption configurations of the NO_2 molecule adsorbed on γ-PC.

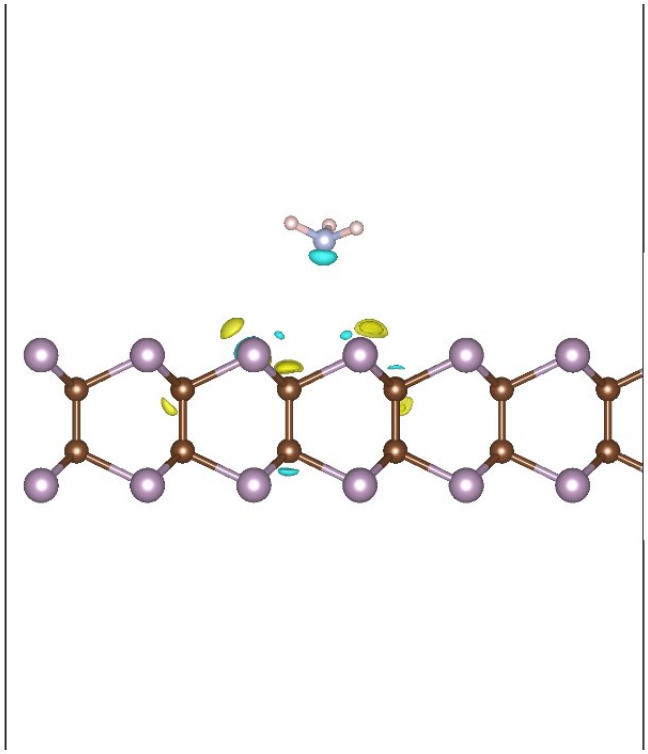

Figure S4. The DCD isosurface plots (10^{-3} Å^{-3}) for the NH_3-adsorbed γ-PC. The yellow (blue) colour represents an accumulation (depletion) of electrons.

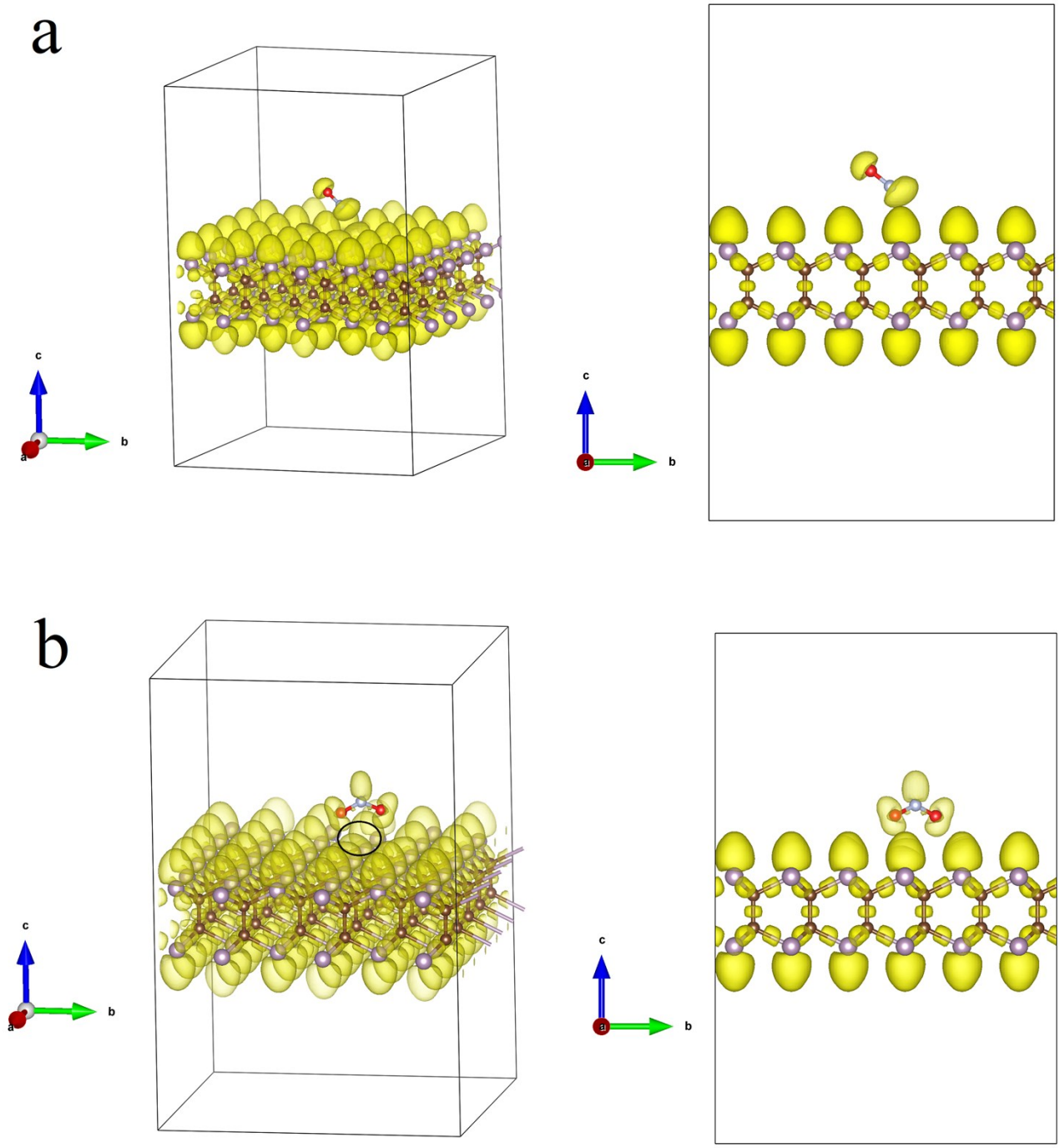

Figure S5. The electronic localization function of (a) NO and (b) NO_2 molecule-adsorbed γ-PC.