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

Supplementary Information for

The interaction of two-dimensional α- and β-phosphorus carbide with environmental molecules: a DFT study

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This PDF file includes:

Figs. S1 to S8

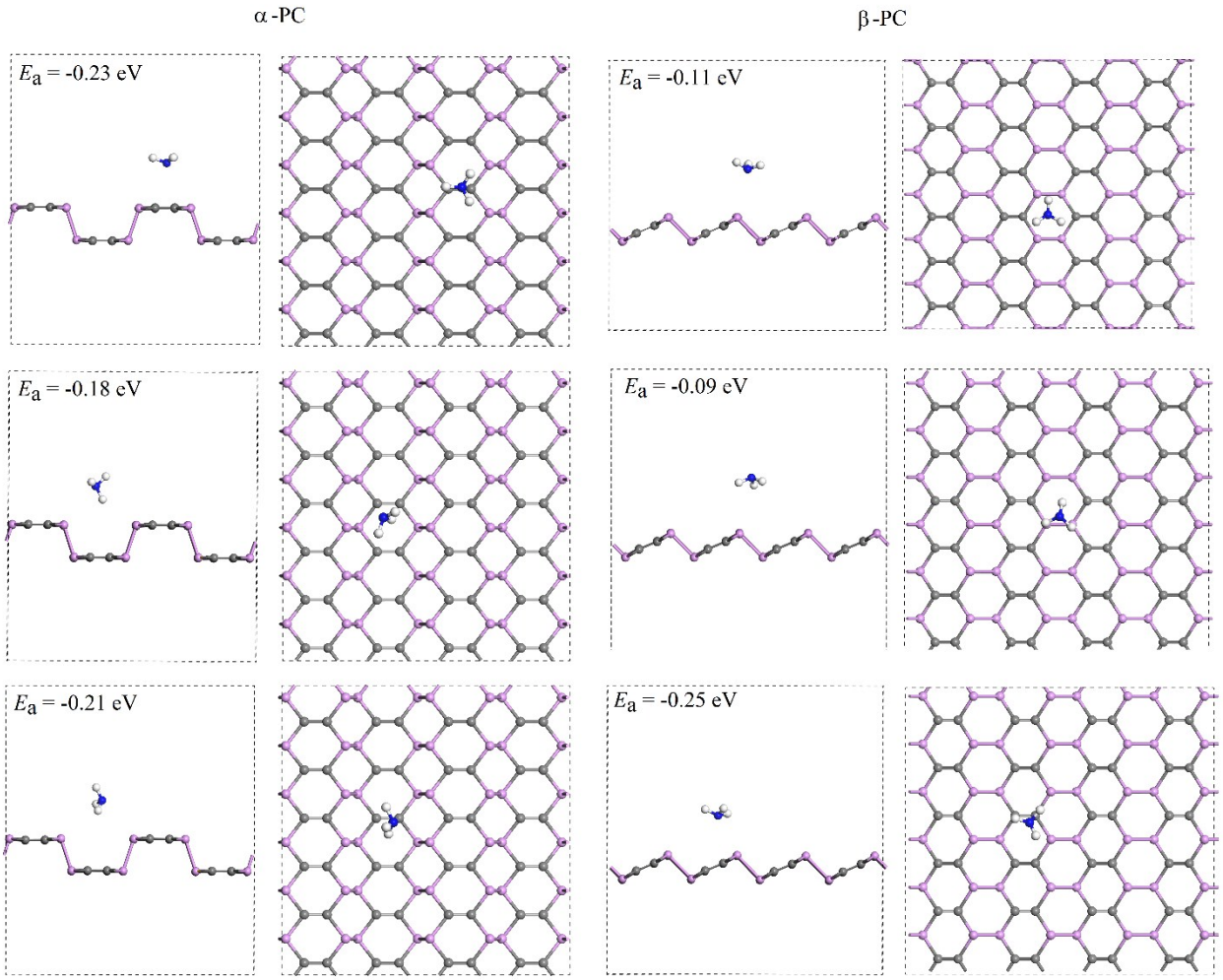

Figure S1. The top and side views of the examined possible absorption configurations of the NH_3 molecule adsorbed on *α*- and *β*-PC.

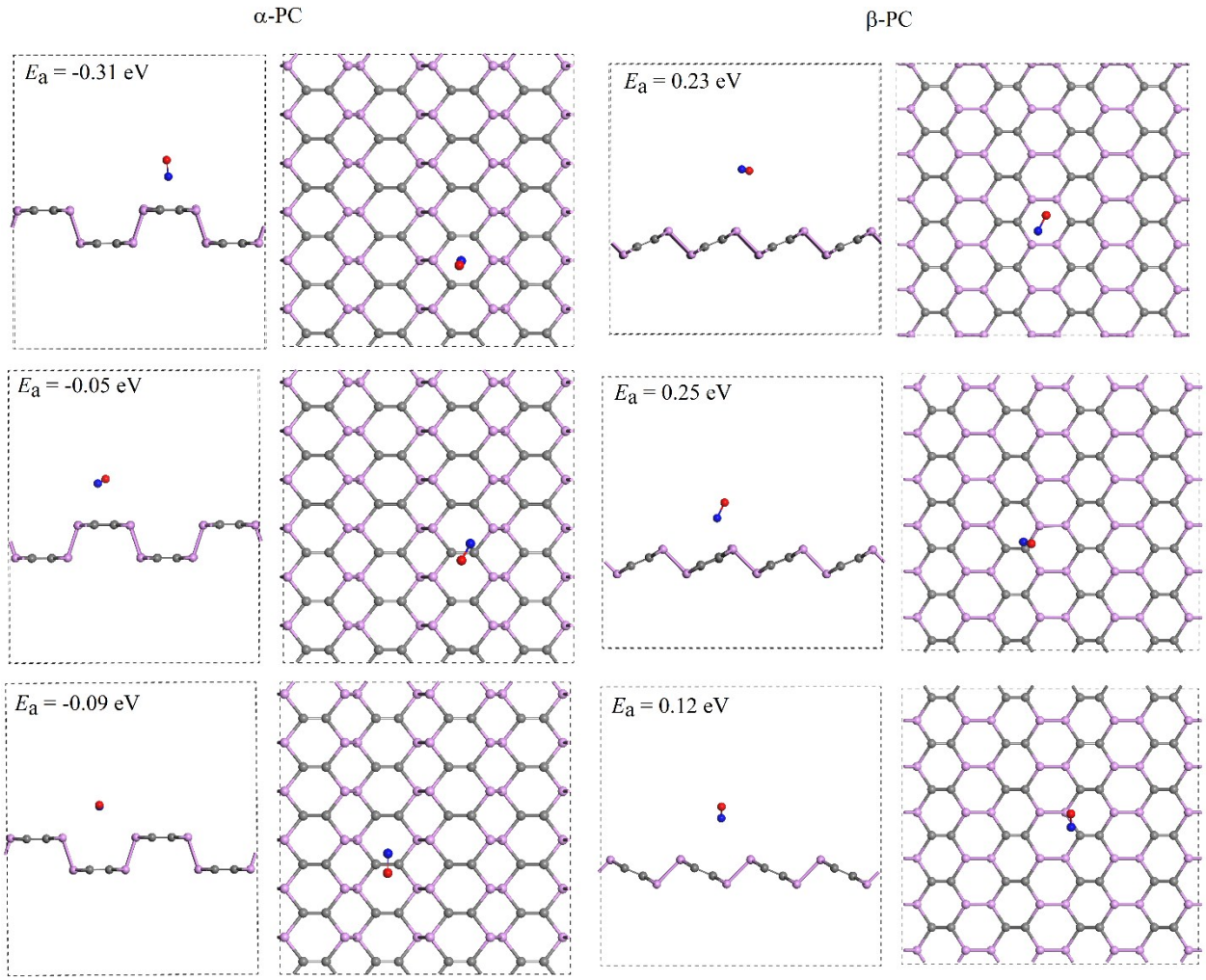

Figure S2. The top and side views of the examined possible absorption configurations of the NO molecule adsorbed on *α*- and *β*-PC.

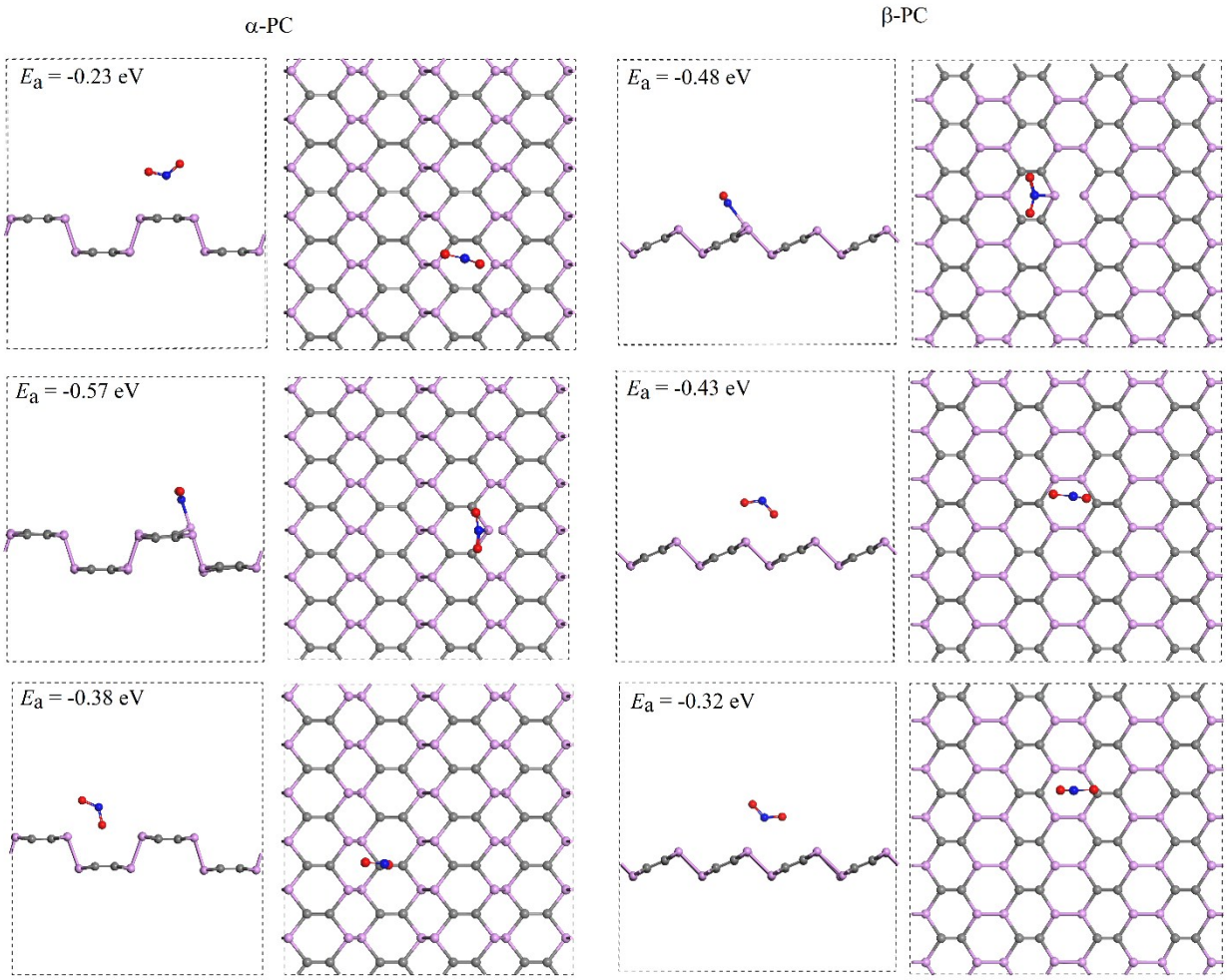

Figure S3. The top and side views of the examined possible absorption configurations of the NO_2 molecule adsorbed on *α*- and *β*-PC.

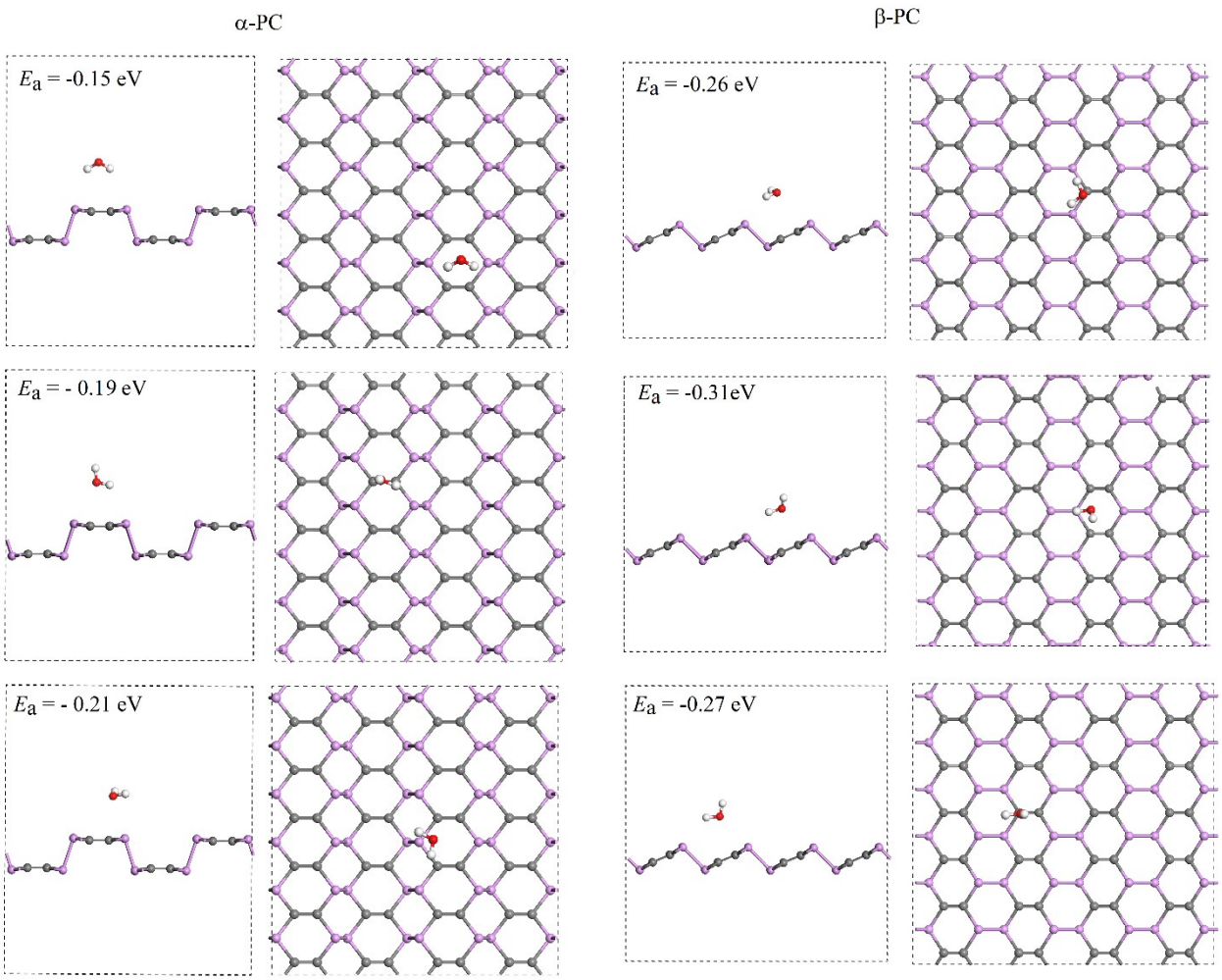

Figure S4. The top and side views of the examined possible absorption configurations of the H_2O molecule adsorbed on *α*- and *β*-PC.

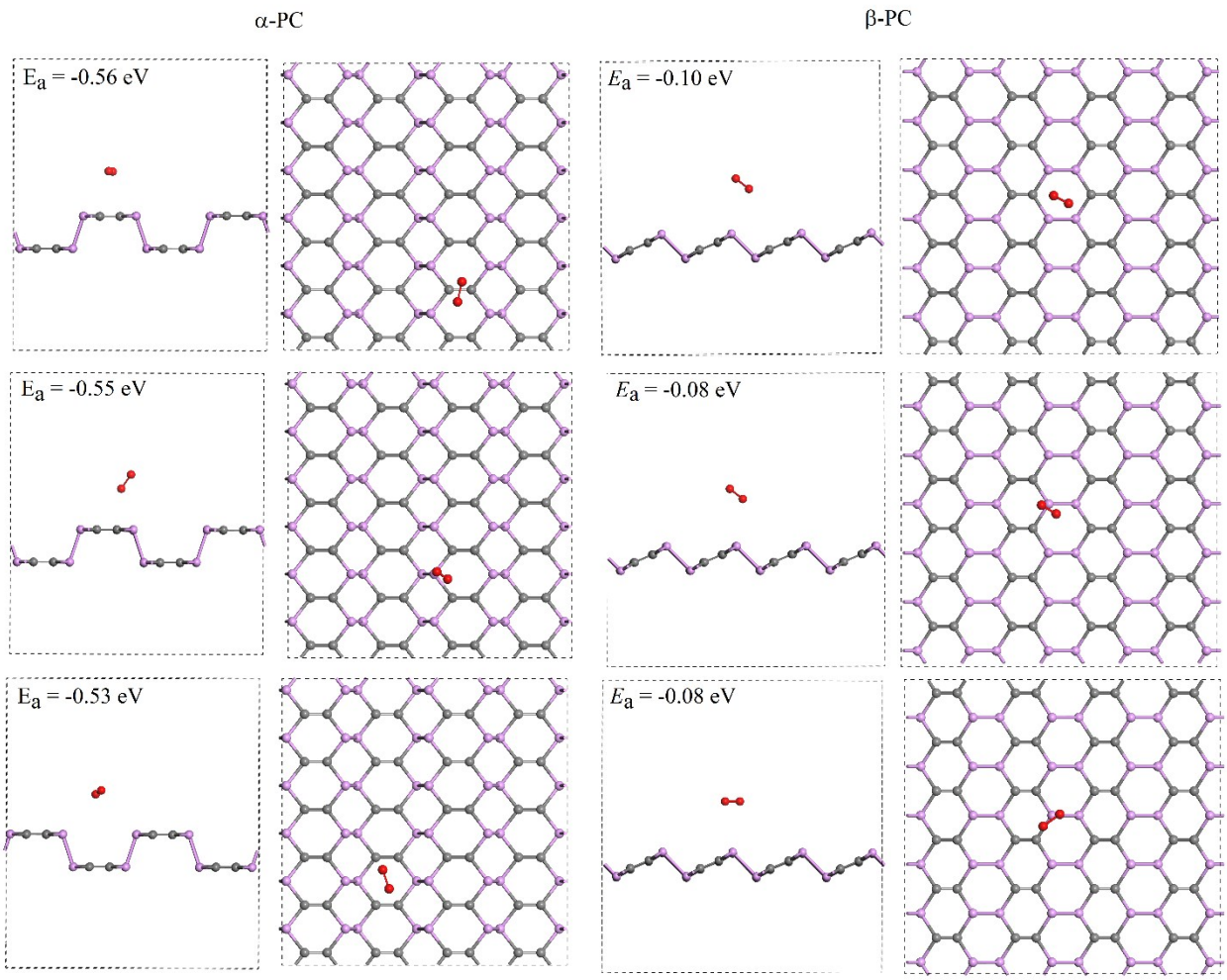

Figure S5. The top and side views of the examined possible absorption configurations of the O_2 molecule adsorbed on *α*- and *β*-PC.

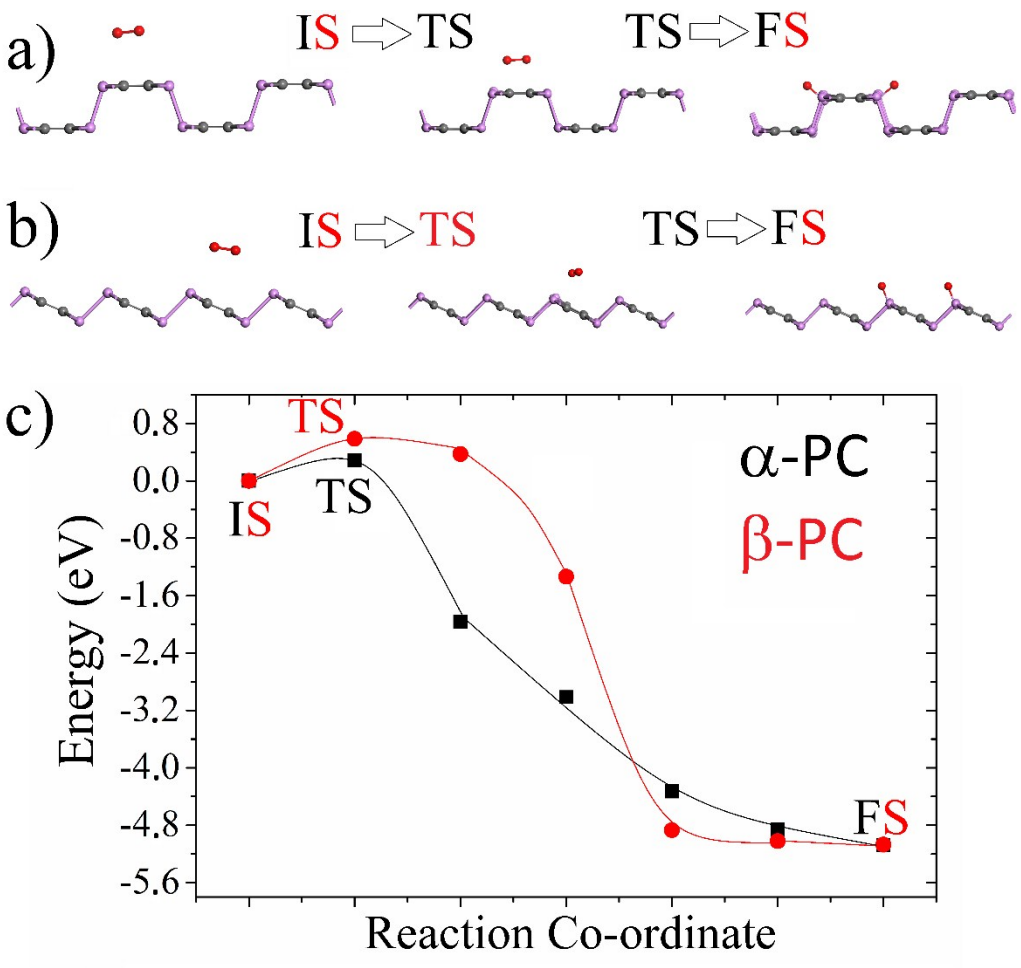

Figure S6. The activation barrier for the O_2 molecule splitting on *α*- and *β*-PC. The atomic models for the initial state (IS), transition state (TS) and final state (FS) for (a) *α*- and (b) *β*-PC. The energy profile obtained by the NEB calculation for the decomposition of the O_2 molecule on *α*- (the black line) and *β*-PC (the red line).

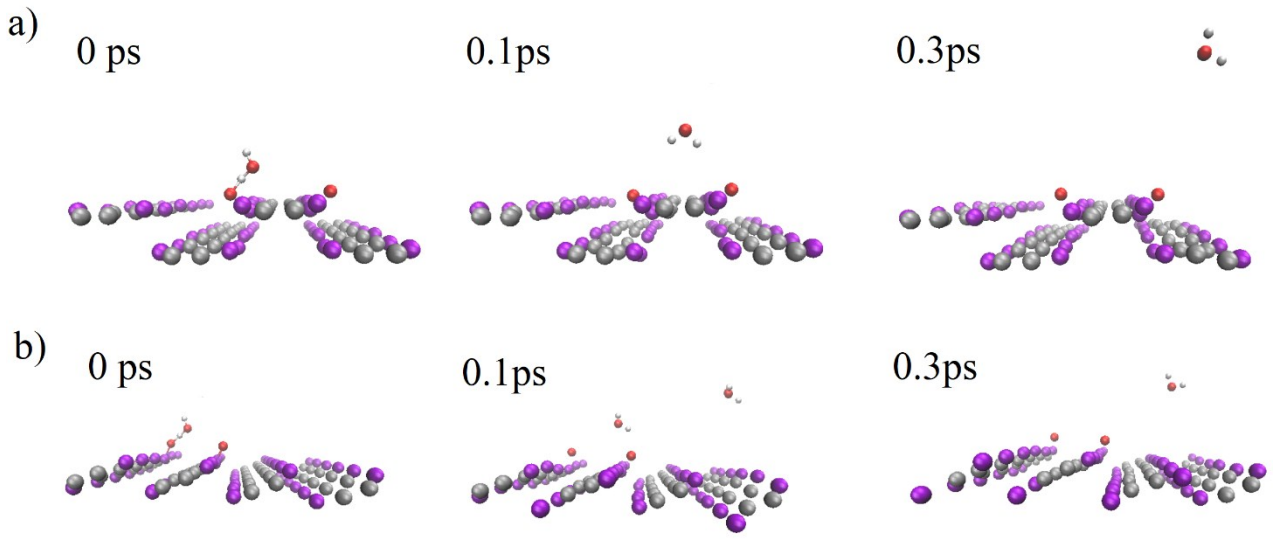

Figure S7. The snapshots of the H_2O motion on pre-oxidized α- and β-PC surfaces calculated by AIMD at 300 K. The P, C, H, and O are coloured in violet, grey, white, and red, respectively.

To show the specific of high sensitivity of PC to environmental gas molecules, as an example, the electronic localization function (ELF) of NO molecule-adsorbed α-PC is calculated (Figure S8). 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 S8. It can be seen that a significant number of electrons are distributed between the C-C and the C-P bonds, indicating a strong covalent bonging between carbon atoms and carbon and phosphorus atoms. In addition, a strong charge localization is observed on phosphorus atoms. This allows strong charge transfer from the phosphorus atoms to external molecules. This is also seen in Figure S8 (the black circle on the left panel) a strong charge depletion of the phosphorus atom which is nearby the NO molecule and the charge accumulation on the nitrogen and oxygen atoms of the molecule is observed.

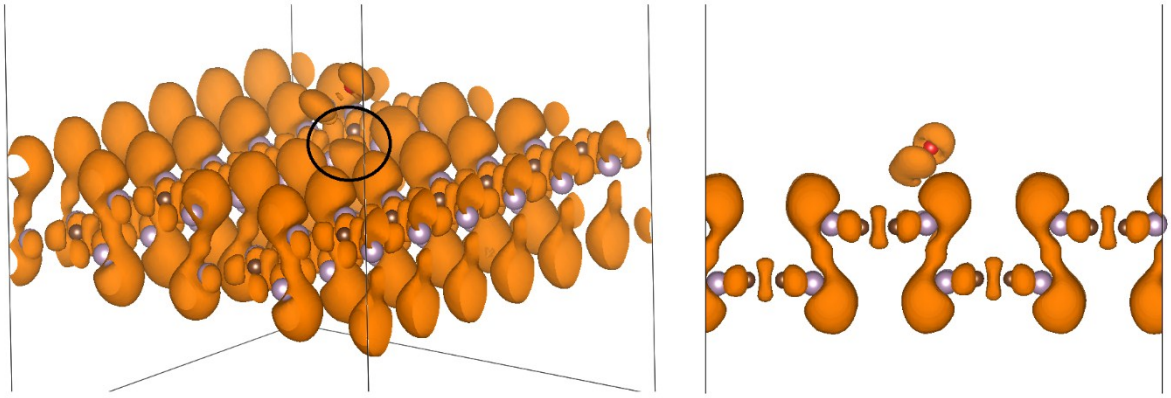

Figure S8. The electronic localization function (ELF) of NO molecule-adsorbed α-PC.