Electronic Supplementary Information

The impact of metalation on adsorption geometry, electronic level alignment and UV-stability of organic macrocycles on TiO_2(110)

Manuel Graf[1,2], Gerson Mette[1,3,*], Dominik Leuenberger[1], Yeliz Gurdal[4], Marcella Iannuzzi[4], Wolf-Dietrich Zabka[1], Stephan Schnidrig[4], Benjamin Probst[4], Jürg Hutter[4], Roger Alberto[4], and Jürg Osterwalder[1,*]

[1]Physik-Institut, Universität Zürich, CH-8057 Zürich, Switzerland

[2]Present address: Empa, Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

[3]Present address: Fachbereich Physik, Philipps-Universität Marburg, D-35037 Marburg, Germany

[4]Institut für Chemie, Universität Zürich, CH-8057 Zürich, Switzerland

* corresponding authors: Gerson Mette, E-mail: gerson.mette@physik.uni-marburg.de and Jürg Osterwalder, E-mail: osterwal@physik.uzh.ch

1 Photoelectron spectroscopy

1.1 Oxidation state of incorporated Co

The incorporation of Co atoms into the pyrphyrin macrocycle is clearly observable in the Co $2p$ XP-spectrum as depicted in Fig. S1. Right after Co-deposition, the Co(0)-assigned peaks at 778.5 eV and 794 eV for Co $2p_{3/2}$ and Co $2p_{1/2}$, respectively, are pronounced. Thermal annealing results in a transfer of intensity from these peaks into enhanced features at higher binding energy corresponding to an increased oxidation state due to an incorporation into the Pyr molecules.

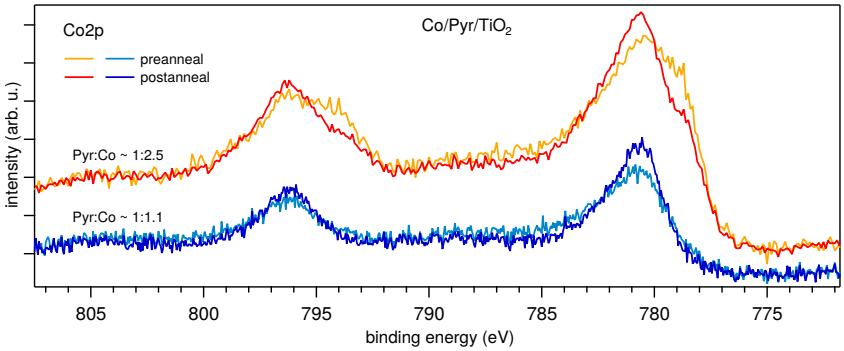

Figure S1: Co 2*p* spectra of in-situ metalated CoPyr on TiO_2 (110) for two different ratios of deposited Co atoms per Pyr molecule before and after annealing.

1.2 Thermal and UV-stability of Pyr on TiO_2(110)

Pyrphyrin on TiO_2(110) does not sustain elevated temperatures of 563 K in its original configuration as shown in Fig. S2. Interestingly, this temperature is below the evaporation temperature of 579 K used for vapor deposition. Hence, TiO_2 seems to have a certain catalytic influence on this process. In the N 1*s* spectrum the most evident change is the decrease of the NH-associated peak, together with an increase in intensity at lower binding energy. We assign this to a deprotonation of the central nitrogen-atoms.

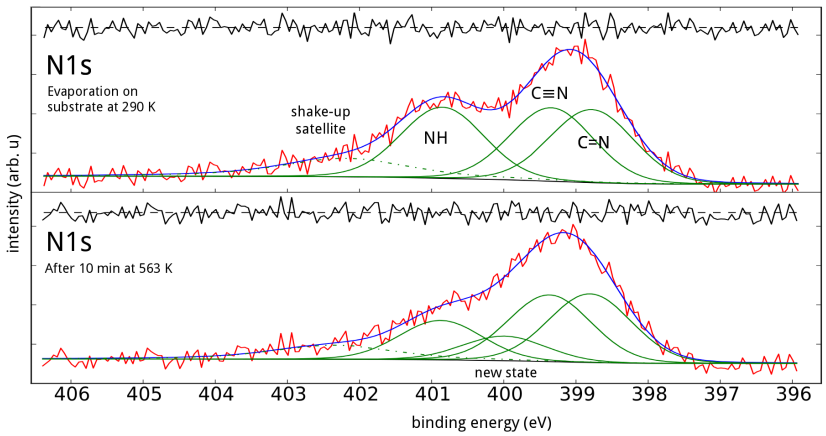

Figure S2: The effect of 10 min annealing at 563 K on the N 1*s* spectrum. The N 1*s* signal is decomposed according to the present chemical species. In each frame, the topmost black curves denote the residuals of the fit.

Continuous UV-irradiation of Pyr/TiO_2(110) is found to induce a rapid and monotonous decrease of the molecule-related UPS signals. Fig. S3a shows the corresponding changes of the N 1*s* core level spectrum due to the UV-irradiation. The observed spectral changes indicate a more complex decomposition of the molecule as the UV-induced degradation affects pyridinic as well as iminic and/or cyano nitrogen bonds of the bare ligand.

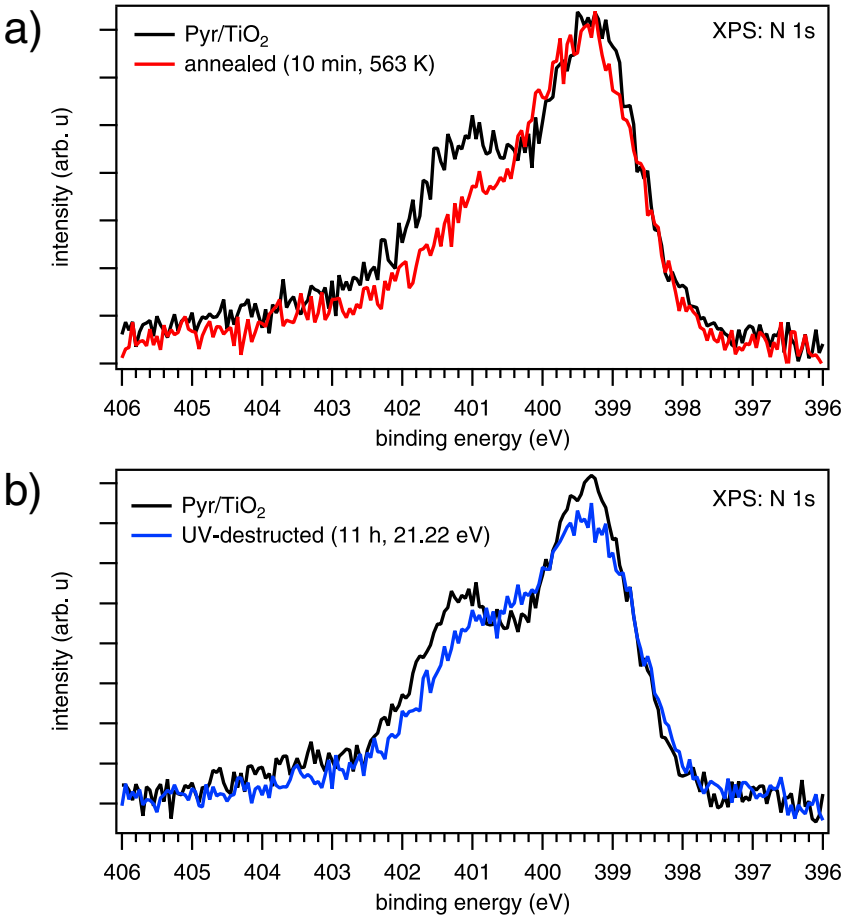

Figure S3: Comparison of the N 1*s* spectra before and after a 10 min annealing of Pyr/TiO_2 at 579 K (a) with the spectra before and after exposure to UV-radiation on Pyr/TiO_2 (b).

1.3 UV-stability of externally prepared CoPyr on TiO_2(110)

For the Co-metalated Pyr molecules an enhanced UV-stability is found. In order to exclude side reactions due to the in-situ metalation procedure, a reference experiment with externally prepared CoPyr was performed. Here, CoPyr is directly evaporated onto the TiO_2(110) surface.

Fig. S4 shows the UP-spectra before and after an exposure to UV-irradiation for 27 min. In agreement with the results of the in-situ prepared CoPyr, no UV-induced degradation is observed for the externally prepared CoPyr on TiO_2. Thus, side reactions due to the metalation procedure can be excluded. Please note, that the small increase of the intensity after the exposure can be attributed to a slight increase of the photon flux of the UV-source.

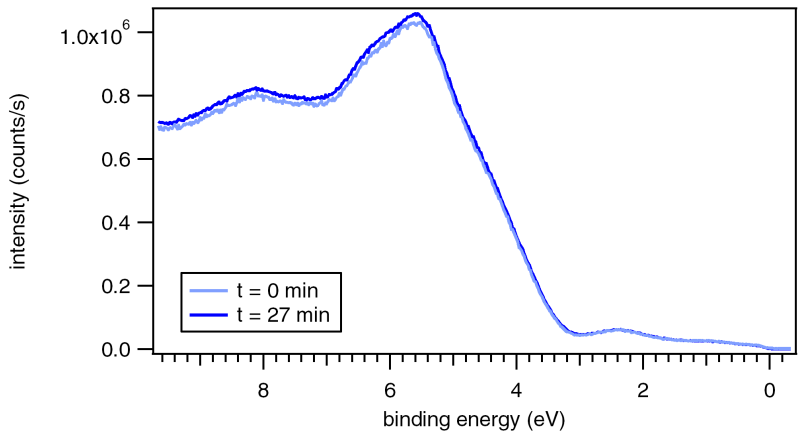

Figure S4: UP-spectra of externally prepared CoPyr/TiO_2(110) before and after exposure to He Iα radiation (21.2 eV) for 27 min.

1.4 Semiconductor band bending on Pyr adsorption

A gradual shift to higher binding energy is found for the valence band maximum as a function of the Pyr coverage as shown in Fig. S5.

1.5 Work function dependence on coverage

With increasing Pyr coverage the work function changes significantly from $\Phi_{clean} = 4.9 \pm 0.1$ eV on clean TiO_2(110) to a minimum of $\Phi_{Pyr} = 3.7 \pm 0.1$ eV at 0.75 ML Pyr coverage as shown in Fig. S6. For longer Pyr exposures, larger values of the work function are again found. The work function of CoPyr does not change significantly with respect to Pyr ($\Phi_{CoPyr} = 3.8 \pm 0.1$ eV).

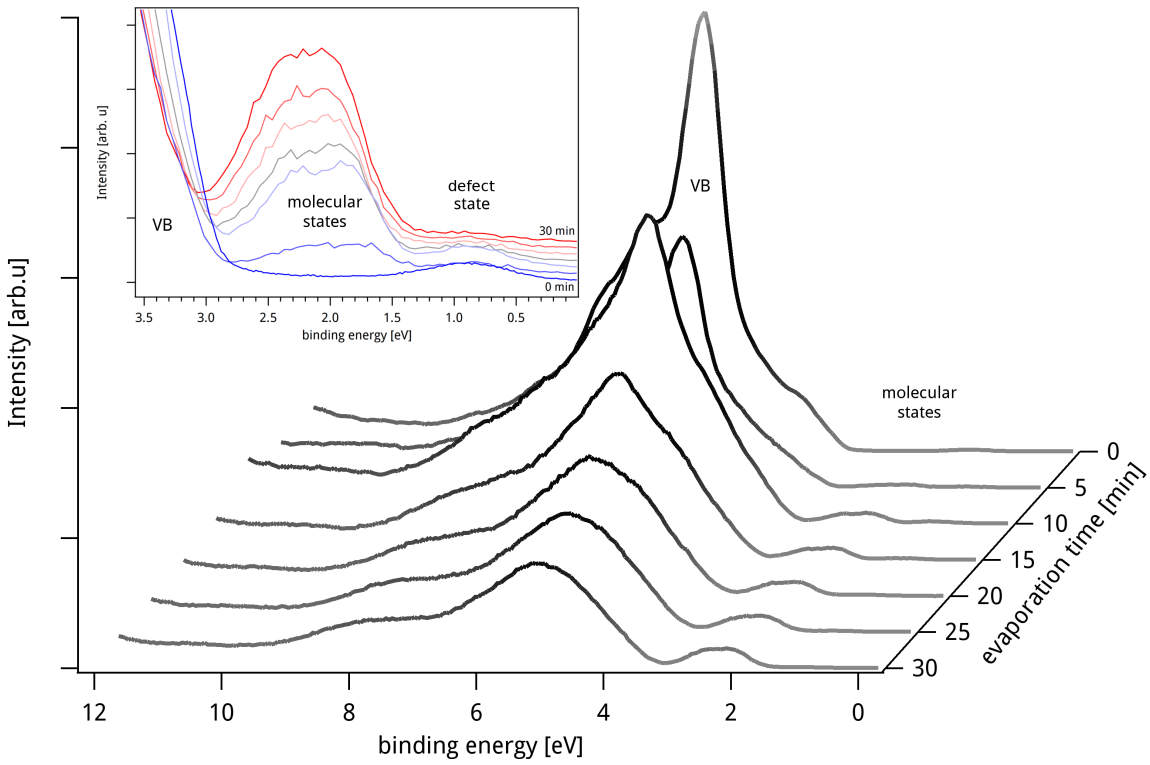

Figure S5: Coverage dependent UP-spectra of Pyr/TiO_2. The inset is a close-up of the bandgap region.

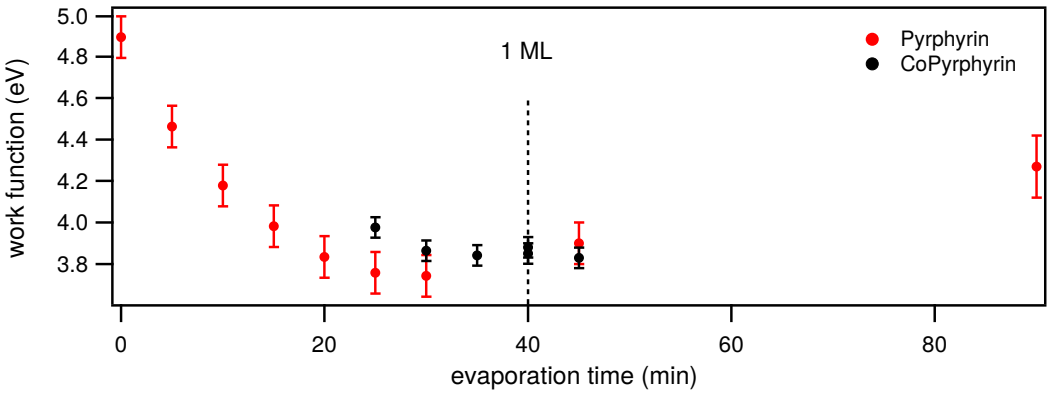

Figure S6: Coverage dependent work function change of Pyr and CoPyr on TiO_2(110).

2 DFT calculation

2.1 Computational details

The adsorbed molecules on the TiO_2(110) surface are simulated employing a slab model, where the oxide is represented by five O-Ti-O layers, plus 20 Å of vacuum to avoid interactions with the periodic images in the (110) direction. While monomer calculations are carried out using a 7×3×5 TiO_2 slab, for the monolayer calculations a 8×2×5 TiO_2 slab is used. In both cases, the two topmost layers of the slab are relaxed, whereas the rest is kept fixed in the bulk positions. As it is discussed in detail in our previous work [1], the five atomic layer slab model accurately captures the properties of TiO_2(110) surface. Pyrphyrin is always adsorbed flat on the oxide surface and several possible orientations of the molecule were tested in order to determine the most stable configuration. The electronic structure distribution is investigated by means of the projected densities of states. The simulation of the STM images are carried out using the Tersoff–Hamann approximation [2].

Monomer and monolayer structures on the TiO_2(110) surface are characterized by different energies and structural parameters. The adsorption energy, E_{ads}, is calculated as

$$E_{\mathrm{ads}} = [E_{\mathrm{complex}} - (E_{\mathrm{slab}} + n_{mol} E_{\mathrm{monomer}})]/n_{mol} \tag{1}$$

where E_{complex} is the total energy of the optimized complex, E_{slab} is the energy of the slab, and E_{monomer} is the energy of the free standing molecule. For the monomer calculations n_{mol} is 1, whereas it is equal to 2 for the monolayer case. The amount of dispersion energy, E_{disp}, is calculated in a similar way like E_{ads}.

$$E_{\mathrm{disp}} = [E^{\mathrm{disp}}_{\mathrm{complex}} - \left(E^{\mathrm{disp}}_{\mathrm{slab}} + n_{mol} E^{\mathrm{disp}}_{\mathrm{monomer}}\right)]/n_{mol} \tag{2}$$

For the monolayer adsorption on the TiO_2(110) surface the stability of the complexes, both Pyr/TiO_2 and CoPyr/TiO_2, are evaluated in terms of three parameters: the molecules–substrate interactions ($E^{\mathrm{monolayer}}_{\mathrm{int}}$), the distortion energy of the monolayer ($E^{\mathrm{monolayer}}_{\mathrm{dist}}$), and the intermolecular interactions ($E^{\mathrm{inter}}_{\mathrm{mol}}$) which are calculated as

$$E^{\mathrm{monolayer}}_{\mathrm{int}} = [E_{\mathrm{complex}} - (E_{\mathrm{monolayerd}} + E_{\mathrm{slabd}})]/n_{\mathrm{mol}} \tag{3}$$

$$E_{\text{dist}}^{\text{monolayer}} = [E_{\text{monolayerd}} - E_{\text{monolayer}}]/n_{\text{mol}} \quad (4)$$

$$E_{\text{mol}}^{\text{inter}} = [E_{\text{monolayer}} - n_{\text{mol}} E_{\text{monomer}}]/n_{\text{mol}} \quad (5)$$

respectively. E_{slabd} is the energy of the bare slab at the coordinates of the complex, $E_{\text{monolayer}}$ is the energy of the monolayer computed as free standing, and $E_{\text{monolayerd}}$ is the energy calculated in vacuo with the same coordinates of the monolayer in the complex.

2.2 Monomer adsorption on TiO_2(110)

2.2.1 Geometry optimization

The resulting optimized complex of Pyr/TiO_2(110) is shown in Figure S7. E_{ads} is calculated as -4.22 eV, indicating relatively strong interactions between Pyr and TiO_2. Apart from chemical interactions, van der Waals interactions contribute significantly by $E_{\text{disp}} = -2.57$ eV. The distance between cyano-N and five-coordinated surface Ti atom becomes 2.14 Å. The convex shape of the molecule on the oxide surface due to this bonding of cyano-N with the surface Ti atoms results in a cyano-N–cyano-N distance of 10.98 Å compared to 11.96 Å in the gas phase.

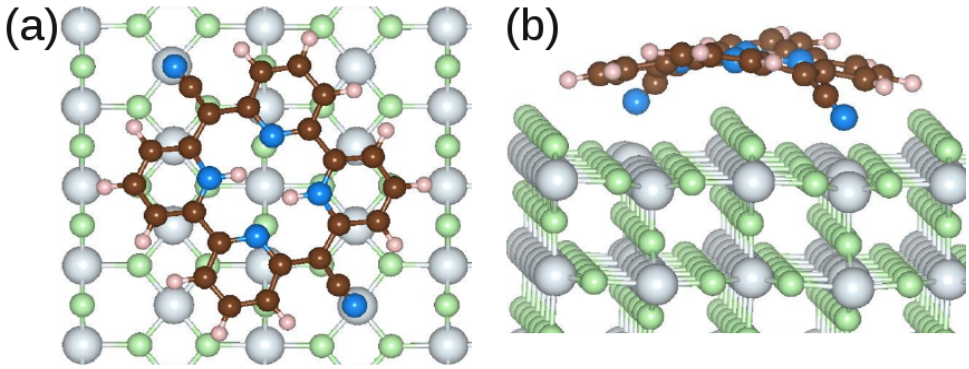

Figure S7: Top view (a) and side view (b) of the optimized structure of Pyr on TiO_2(110). For clarity only the surface layer and two rutile layers are shown in a and b, respectively. Color code: blue: N, brown: C, pink: H, green: O, and gray: Ti.

Apart from this structure, an alternative configuration is possible where the two protons attached to the pyridinic nitrogens are closer to the two-coordinated surface oxygens. The optimized structure of this alternative configuration is shown in Figure S8. The adsorption energies

of the two configurations are almost the same, the difference is only around 0.09 eV. In contrast, to the observation for tetraphenylporphyrin on TiO_2(110) [3], we do not observe bending of the protons attached to the pyridinic nitrogen atoms towards the surface oxygen atoms. The proton–pyridinic-nitrogen bond lengths are almost the same in the two configurations, around 1.04 Å.

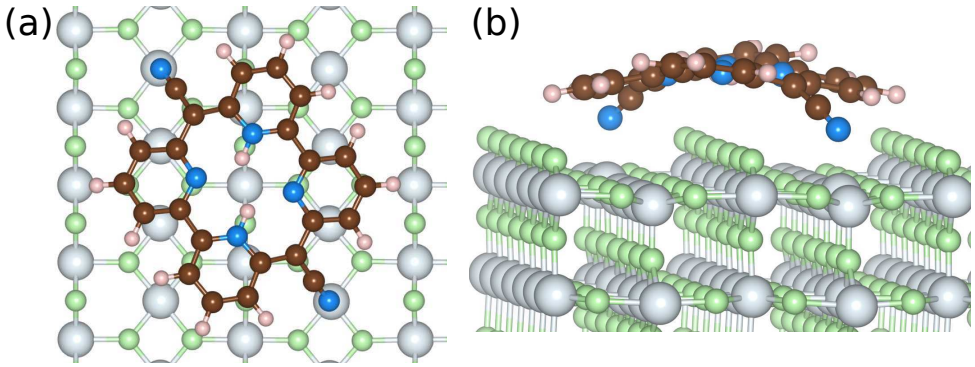

Figure S8: Alternative configuration of Pyr/TiO_2(110) where the protons attached to the pyridinic nitrogens are positioned on top of the two-coordinated surface oxygen atoms. Top view and side view are shown in (a) and (b), respectively. Color code: see the previous figure.

2.2.2 Electron density difference

A Bader charge analysis [4] is carried out for the optimized configurations of Pyr/TiO_2 and CoPyr/TiO_2 to shed light on the charge transfer between the molecules and the substrate. Our results show that there is a charge flow from the molecules to the TiO_2 surface which is very similar for Pyr ($0.481e$) and CoPyr ($0.488e$). The charge redistribution can be analyzed by charge density differences.

The electron density difference maps are obtained by calculating $\Delta\rho(\mathbf{r})$,

$$\Delta\rho(\mathbf{r}) = \rho_{\text{complex}}(\mathbf{r}) - (\rho_{\text{slab}}(\mathbf{r}) + \rho_{\text{mol}}(\mathbf{r})). \tag{6}$$

In the above expression, $\rho_{\text{complex}}(\mathbf{r})$ is the total density of the complex, whereas ρ_{slab} and ρ_{mol} are the electron densities of the rutile slab and the Pyr molecule, respectively, at the same coordinates as in the complex.

Figure S9 shows the two isosurfaces of $\Delta\rho(\mathbf{r})$ corresponding to $+0.002$ e/Å^3, i.e., charge accumulation (left panel), and -0.002 e/Å^3 , i.e., charge depletion (right panel). In particular, electron accumulation is observed between cyano-N and the closest under-coordinated Ti atoms. This picture confirms the presence of chemical interactions between cyano-N and five-coordinated Ti species. For an electron density difference analysis of CoPyr/TiO_2, we refer to our previous study [1].

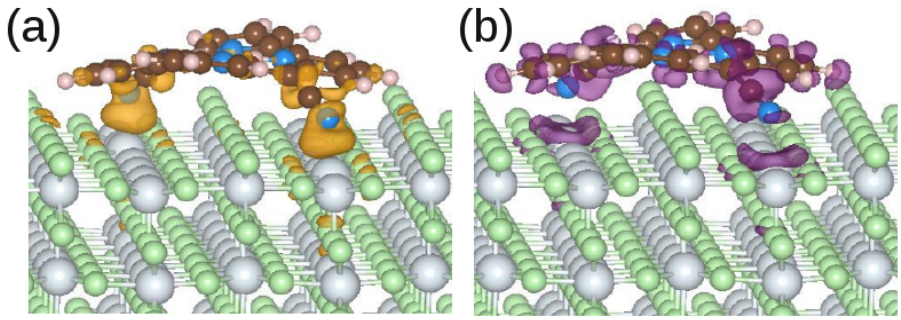

Figure S9: Electron density difference $\Delta\rho(\mathbf{r})$: Isosurfaces correspond to 0.002 e/Å^3 (a) and -0.002 e/Å^3 (b).

2.2.3 Molecular orbitals of Pyr

Figure S10 shows the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of Pyr in the gas phase. The molecular orbitals are distributed over all pyridine rings.

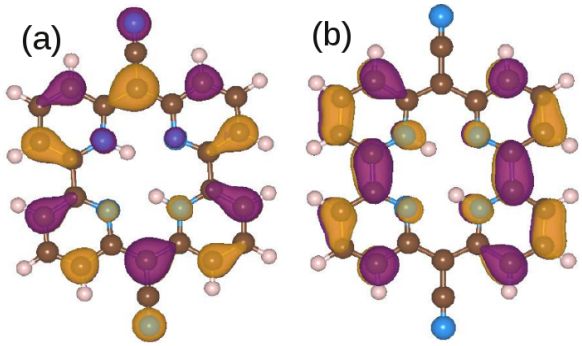

Figure S10: Selected molecular orbitals of optimized Pyr in the gas phase, (a) HOMO and (b) LUMO. Color code: brown: C, blue: N, and light pink: H. Isosurface (orange for positive and purple for negative) is set to ± 0.03 e/Å^3.

2.2.4 Molecular orbital of Pyr/TiO_2(110)

Figure S11 shows the HOMO of the Pyr/TiO_2(110) complex. As a general observation, the HOMO is a molecular state of Pyr and extends in the region between molecule and surface.

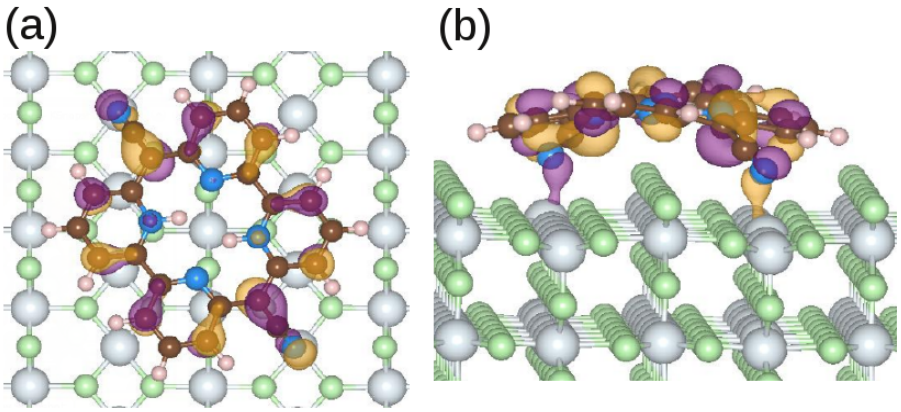

Figure S11: Representation of the HOMO of Pyr adsorbed on TiO_2(110). Top (a) and side (b) view. The displayed isosurfaces (orange for positive and purple for negative) are obtained at ± 0.036 e/Å^3.

2.2.5 Comparison of neutral and charged molecules

Electronic redistribution of neutral and negatively ($-1e$) charged Pyr and CoPyr molecules in vacuo is compared. The level alignment is carried out with respect to the lowest energy molecular orbital of neutral molecules. The DFT results show that the HOMO-LUMO gap of Pyr^- (0.26 eV) is significantly narrower than that of neutral Pyr (2.23 eV). The HOMO of Pyr^- becomes 1.41 eV less stable than the HOMO of Pyr. Additionally, the difference of HOMO and HOMO-1 states becomes more significant in Pyr^-. While HOMO and HOMO-1 show an energy difference of 1.81 eV in Pyr^-, it is only 0.5 eV in Pyr.

For $CoPyr^-$ we do not observe significant changes of the HOMO-LUMO gap or in the difference of HOMO and HOMO-1. Our calculations show that the singlet state of $CoPyr^-$ is more stable than the triplet state by 0.46 eV. Therefore, further calculations were carried out using a singlet spin state. The HOMO-LUMO gaps are calculated as 1.57 eV and 2.02 eV for $CoPyr^-$ and neutral CoPyr, respectively. Contrary to the Pyr^- case, the HOMO of $CoPyr^-$ becomes 1 eV

more stable than its neutral counterpart. While the HOMO and HOMO-1 difference is 0.21 eV in $CoPyr^-$, it is 0.72 eV in CoPyr. A Bader charge analysis [4] shows that charges localize on the Co center for CoPyr in vacuo and similarly for $CoPyr/TiO_2$ (around $+1.02e$). In comparison, the Co center has $+0.71e$ of charge for the $CoPyr^-$ molecule at vacuum.

2.3 Monolayer calculations

2.3.1 Pyr monolayer on TiO_2(110)

As it is mentioned in the main article, LEED results suggest a distorted $c(8 \times 2)$ superstructure for 1 ML of Pyr on TiO_2(110). Figure S12 shows the optimized $c(8 \times 2)$ superstructure of a Pyr monolayer on the TiO_2(110) surface. Geometry optimization exhibits that the molecules preserve their convex shape towards the surface as suggested by the monomer calculations.

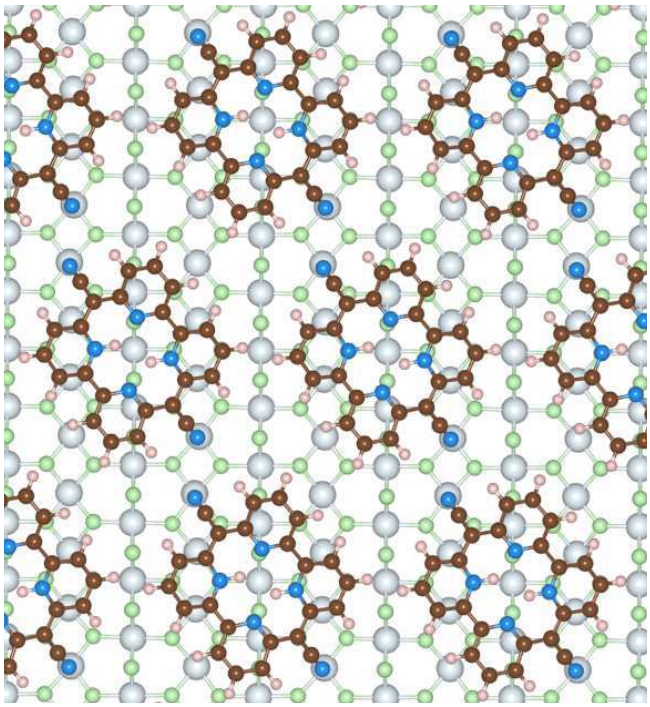

Figure S12: Optimized $c(8 \times 2)$ Pyr monolayer configuration on TiO_2 (110). For clarity only the surface layer of TiO_2(110) is depicted. Color code: see the previous figures.

E_{ads} is calculated as -3.76 eV which is slightly lower than in the monomer case. Instead, E_{disp} is calculated as -2.73 eV being slightly larger than for the isolated monomer. While

the molecules–substrate interaction, $E_{\text{int}}^{\text{monolayer}}$, is computed as -5.26 eV, the term for the intermolecular interactions, $E_{\text{mol}}^{\text{inter}}$, is calculated as -0.51 eV. As in the monomer case, cyano-N of each Pyr molecule is well positioned on the surface Ti atoms with a measured distance of ≈2.2 Å. The smallest distance between two cyano nitrogens of two Pyr molecules becomes 3.1 Å. This configuration results in distortion energy of the monolayer, $E_{\text{dist}}^{\text{monolayer}}$, to be 1.13 eV.

2.3.2 CoPyr monolayer on TiO_2(110)

The optimized $c(8 \times 2)$ superstructure of a CoPyr monolayer on the TiO_2 (110) surface is shown in Figure S13. Again, the CoPyr molecules preserve their bent shape also in the monolayer case. E_{ads} and E_{disp} contributions are computed as -3.73 eV and -2.83 eV, respectively. Compared to the results of the isolated monomer [1], the monolayer calculations give slightly lower and larger E_{ads} and E_{disp}, respectively.

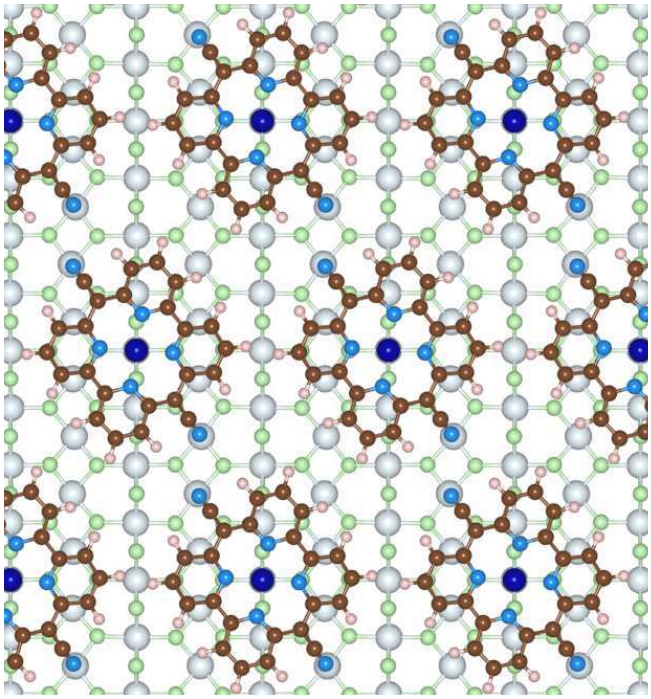

Figure S13: Optimized $c(8 \times 2)$ CoPyr monolayer configuration on TiO_2 (110). For clarity only the surface layer of TiO_2(110) is depicted. Color code: see the previous figures.

The distance between the two cyano-N atoms of the same CoPyr molecule is 10.87 Å which is very similar to the monomer adsorption case. The distance between cyano-N and the under-

coordinated Ti becomes 2.2 Å which is slightly larger than for the CoPyr monomer adsorption (2.13 Å). The molecules–substrate interaction, $E_{\mathrm{int}}^{\mathrm{monolayer}}$, is computed as −5.35 eV for this configuration. The shortest distance between two cyano-N atoms of two adjacent CoPyr molecules becomes 3.2 Å. The computed $E_{\mathrm{dist}}^{\mathrm{monolayer}}$ and $E_{\mathrm{mol}}^{\mathrm{inter}}$ are 1.15 eV and −0.48 eV, respectively.

2.3.3 TDOS of Pyr and CoPyr monolayer on TiO_2

The densities of states (DOS) projected on the two molecules and on their substrates, respectively, are already shown in the main text for the bandgap region. Figure S14 shows the total density of states (TDOS) of Pyr and CoPyr monolayers on TiO_2 in comparison with their molecular PDOS and for a larger energy region. The spectra are aligned to the valence band onsets of the corresponding experimental spectra as shown in the main text.

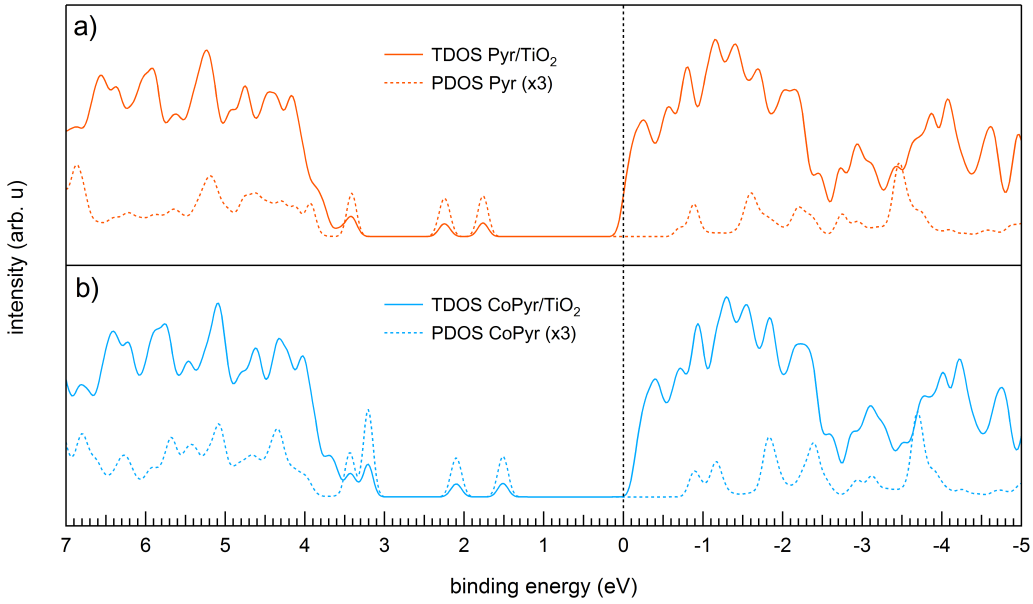

Figure S14: (a) TDOS of Pyr/TiO_2 and (b) $CoPyr/TiO_2$ in comparion to their molecular PDOS.

2.4 Optimized Coordinates

Cartesian coordinates (in Å) for DFT-optimized geometries of the surface structures in our electronic structure calculations.

Table S1: CoPyr monomer on rutile TiO_2 (110) surface.

Table S2: Pyr monomer on rutile TiO_2 (110) surface.

Table S3: CoPyr monolayer on rutile TiO_2 (110) surface.

Table S4: Pyr monolayer on rutile TiO_2 (110) surface.

Table S1: CoPyr monomer on rutile TiO_2 (110) surface

Co	-3.222	-1.491	10.394	N	-5.115	-1.302	10.341	N	-2.850	0.373	10.508
N	-3.596	-3.355	10.499	N	-1.328	-1.680	10.361	N	-6.394	2.920	8.762
N	-0.053	-5.897	8.765	C	-7.214	-0.197	9.909	C	-7.885	-1.404	9.927
C	-7.168	-2.581	10.160	C	-5.797	-2.498	10.373	C	-5.813	-0.144	10.124
C	-5.131	1.131	10.093	C	-5.806	2.144	9.439	C	-3.754	1.394	10.448
C	-3.324	2.729	10.634	C	-1.982	3.021	10.792	C	-1.051	1.979	10.730
C	-1.513	0.676	10.579	C	-4.933	-3.659	10.552	C	-5.396	-4.963	10.693
C	-4.465	-6.004	10.767	C	-3.121	-5.711	10.632	C	-2.690	-4.375	10.448
C	-1.311	-4.111	10.104	C	-0.637	-5.122	9.446	C	-0.629	-2.836	10.141
C	-0.648	-0.483	10.401	C	0.724	-0.399	10.193	C	1.443	-1.574	9.952
C	0.772	-2.782	9.928	H	-7.762	0.725	9.721	H	-8.954	-1.438	9.730
H	-7.673	-3.544	10.137	H	-4.066	3.524	10.617	H	-1.656	4.051	10.923
H	0.016	2.177	10.798	H	-6.464	-5.162	10.739	H	-4.792	-7.035	10.888
H	-2.379	-6.506	10.623	H	1.228	0.564	10.175	H	2.511	-1.538	9.752
H	1.320	-3.702	9.731	O	3.294	-0.005	7.826	O	-9.750	-0.003	7.811
O	-3.239	-0.010	7.770	O	3.300	-2.958	7.818	O	-9.736	-2.954	7.822
O	-3.218	-2.950	7.772	O	3.265	-5.925	7.816	O	-9.733	-5.923	7.836
O	-3.193	-5.915	7.780	O	3.295	-8.895	7.823	O	-9.731	-8.893	7.830
O	-3.216	-8.887	7.822	O	3.295	8.896	7.826	O	-9.734	8.901	7.826
O	-3.220	8.896	7.832	O	3.292	5.929	7.831	O	-9.731	5.931	7.822

O	-3.224	5.917	7.828	O	3.291	2.963	7.835	O	-9.719	2.965	7.812
O	-3.258	2.949	7.782	Ti	6.545	-0.001	6.372	Ti	-6.470	0.008	6.346
Ti	0.040	-0.007	6.362	Ti	6.539	-2.963	6.373	Ti	-6.498	-2.955	6.360
Ti	0.010	-2.971	6.353	Ti	6.563	-5.929	6.375	Ti	-6.469	-5.921	6.371
Ti	0.076	-5.956	6.636	Ti	6.548	-8.899	6.377	Ti	-6.485	-8.893	6.371
Ti	0.019	-8.909	6.355	Ti	6.547	8.900	6.377	Ti	-6.480	8.901	6.360
Ti	0.036	8.894	6.362	Ti	6.545	5.937	6.377	Ti	-6.470	5.946	6.355
Ti	0.035	5.928	6.372	Ti	6.527	2.968	6.375	Ti	-6.528	2.993	6.633
Ti	0.018	2.959	6.372	O	-3.257	0.000	1.256	O	3.257	0.000	1.256
O	-9.771	0.000	1.256	O	-3.257	-2.966	1.256	O	3.257	-2.966	1.256
O	-9.771	-2.966	1.256	O	-3.257	-5.932	1.256	O	3.257	-5.932	1.256
O	-9.771	-5.932	1.256	O	-3.257	-8.898	1.256	O	3.257	-8.898	1.256
O	-9.771	-8.898	1.256	O	-3.257	8.898	1.256	O	3.257	8.898	1.256
O	-9.771	8.898	1.256	O	-3.257	5.932	1.256	O	3.257	5.932	1.256
O	-9.771	5.932	1.256	O	-3.257	2.966	1.256	O	3.257	2.966	1.256
O	-9.771	2.966	1.256	Ti	0.000	0.000	0.000	Ti	6.514	0.000	0.000
Ti	-6.514	0.000	0.000	Ti	-0.000	-2.966	0.000	Ti	6.514	-2.966	0.000
Ti	-6.514	-2.966	0.000	Ti	-0.000	-5.932	0.000	Ti	6.514	-5.932	0.000
Ti	-6.514	-5.932	0.000	Ti	-0.000	-8.898	0.000	Ti	6.514	-8.898	0.000
Ti	-6.514	-8.898	0.000	Ti	0.000	8.898	0.000	Ti	6.514	8.898	0.000
Ti	-6.514	8.898	0.000	Ti	0.000	5.932	0.000	Ti	6.514	5.932	0.000
Ti	-6.514	5.932	0.000	Ti	0.000	2.966	0.000	Ti	6.514	2.966	0.000
Ti	-6.514	2.966	0.000	Ti	0.119	-1.517	3.138	O	0.027	0.007	1.998
O	0.019	0.001	4.555	O	-1.933	-1.484	3.240	O	1.992	-1.481	3.272
Ti	6.634	-1.482	3.188	O	6.534	0.002	2.006	O	6.536	0.002	4.561
O	4.579	-1.482	3.267	O	8.493	-1.487	3.273	Ti	-6.391	-1.447	3.137
O	-6.495	0.025	2.000	O	-6.495	-0.015	4.539	O	-8.457	-1.484	3.265
O	-4.527	-1.477	3.250	Ti	0.114	-4.500	3.275	O	0.026	-2.986	2.001
O	0.023	-2.941	4.545	O	-1.942	-4.443	3.269	O	1.994	-4.442	3.287
Ti	6.631	-4.448	3.188	O	6.536	-2.966	2.005	O	6.533	-2.968	4.562
O	4.580	-4.447	3.262	O	8.496	-4.452	3.277	Ti	-6.389	-4.433	3.199

O	-6.498	-2.969	1.997	O	-6.488	-2.965	4.553	O	-8.456	-4.449	3.271
O	-4.531	-4.446	3.258	Ti	0.117	-7.356	3.274	O	0.024	-5.929	2.021
O	0.034	-5.927	4.592	O	-1.943	-7.413	3.276	O	1.993	-7.415	3.291
Ti	6.630	-7.413	3.191	O	6.536	-5.931	2.006	O	6.535	-5.927	4.564
O	4.580	-7.411	3.268	O	8.496	-7.410	3.285	Ti	-6.394	-7.411	3.174
O	-6.497	-5.925	2.005	O	-6.490	-5.927	4.562	O	-8.454	-7.410	3.272
O	-4.532	-7.412	3.267	Ti	0.117	-10.345	3.140	O	0.023	-8.877	2.005
O	0.016	-8.916	4.551	O	-1.940	-10.380	3.267	O	1.988	-10.381	3.276
Ti	6.631	-10.379	3.190	O	6.537	-8.895	2.008	O	6.533	-8.895	4.566
O	4.578	-10.382	3.270	O	8.496	-10.378	3.284	Ti	-6.386	-10.392	3.201
O	-6.495	-8.899	2.008	O	-6.490	-8.890	4.563	O	-8.455	-10.378	3.273
O	-4.530	-10.381	3.280	Ti	0.123	7.427	3.202	O	0.022	8.893	2.002
O	0.021	8.897	4.559	O	-1.938	7.415	3.272	O	1.985	7.412	3.285
Ti	6.634	7.417	3.191	O	6.535	8.900	2.008	O	6.534	8.898	4.566
O	4.575	7.414	3.272	O	8.494	7.421	3.277	Ti	-6.398	7.380	3.137
O	-6.493	8.904	2.001	O	-6.492	8.898	4.556	O	-8.454	7.416	3.267
O	-4.525	7.417	3.275	Ti	0.122	4.450	3.174	O	0.024	5.940	2.006
O	0.019	5.924	4.564	O	-1.935	4.458	3.256	O	1.986	4.450	3.280
Ti	6.632	4.453	3.190	O	6.533	5.936	2.007	O	6.535	5.933	4.565
O	4.576	4.451	3.272	O	8.493	4.455	3.273	Ti	-6.401	4.394	3.276
O	-6.492	5.912	2.004	O	-6.490	5.958	4.552	O	-8.460	4.457	3.283
O	-4.521	4.458	3.287	Ti	0.126	1.472	3.200	O	0.026	2.966	2.005
O	0.017	2.970	4.562	O	-1.933	1.488	3.247	O	1.987	1.487	3.282
Ti	6.631	1.487	3.187	O	6.533	2.972	2.006	O	6.534	2.971	4.564
O	4.577	1.487	3.269	O	8.492	1.486	3.270	Ti	-6.391	1.538	3.270
O	-6.493	2.973	2.020	O	-6.489	2.969	4.589	O	-8.461	1.485	3.277
O	-4.520	1.485	3.278	Ti	3.360	-0.007	3.381	Ti	3.279	-1.483	6.720
O	3.305	0.005	5.253	O	1.266	-1.468	6.684	O	5.332	-1.481	6.717
Ti	-9.667	0.002	3.371	Ti	-9.739	-1.481	6.712	O	-9.758	-0.001	5.242
O	7.766	-1.486	6.704	O	-7.718	-1.493	6.674	Ti	-3.152	0.011	3.342
Ti	-3.230	-1.484	6.668	O	-3.191	-0.008	5.218	O	-5.273	-1.487	6.715

O	-1.178	-1.477	6.726	Ti	3.349	-2.970	3.374	Ti	3.301	-4.446	6.734
O	3.311	-2.962	5.251	O	1.264	-4.415	6.694	O	5.335	-4.451	6.730
Ti	-9.670	-2.967	3.378	Ti	-9.733	-4.446	6.749	O	-9.743	-2.973	5.250
O	7.772	-4.446	6.711	O	-7.698	-4.450	6.737	Ti	-3.154	-2.956	3.343
Ti	-3.225	-4.447	6.684	O	-3.245	-2.945	5.219	O	-5.260	-4.444	6.715
O	-1.205	-4.411	6.615	Ti	3.357	-5.929	3.386	Ti	3.314	-7.417	6.744
O	3.317	-5.920	5.255	O	1.276	-7.453	6.649	O	5.337	-7.408	6.728
Ti	-9.671	-5.929	3.392	Ti	-9.727	-7.410	6.755	O	-9.726	-5.924	5.263
O	7.776	-7.411	6.707	O	-7.693	-7.407	6.726	Ti	-3.160	-5.930	3.367
Ti	-3.229	-7.423	6.720	O	-3.252	-5.921	5.232	O	-5.258	-7.407	6.725
O	-1.194	-7.440	6.662	Ti	3.350	-8.893	3.387	Ti	3.282	-10.383	6.748
O	3.317	-8.899	5.255	O	1.260	-10.391	6.699	O	5.336	-10.380	6.723
Ti	-9.670	-8.894	3.393	Ti	-9.733	-10.379	6.752	O	-9.724	-8.890	5.260
O	7.775	-10.378	6.703	O	-7.694	-10.373	6.716	Ti	-3.154	-8.899	3.379
Ti	-3.230	-10.388	6.752	O	-3.233	-8.894	5.251	O	-5.254	-10.374	6.709
O	-1.184	-10.390	6.714	Ti	3.358	8.905	3.390	Ti	3.289	7.413	6.750
O	3.304	8.894	5.259	O	1.260	7.405	6.703	O	5.332	7.413	6.719
Ti	-9.667	8.903	3.390	Ti	-9.731	7.418	6.747	O	-9.727	8.900	5.258
O	7.770	7.417	6.713	O	-7.695	7.426	6.712	Ti	-3.153	8.889	3.393
Ti	-3.215	7.406	6.755	O	-3.211	8.899	5.263	O	-5.251	7.424	6.701
O	-1.180	7.406	6.727	Ti	3.358	5.934	3.391	Ti	3.279	4.450	6.753
O	3.300	5.924	5.261	O	1.254	4.444	6.717	O	5.329	4.452	6.721
Ti	-9.673	5.936	3.386	Ti	-9.766	4.456	6.740	O	-9.758	5.944	5.253
O	7.763	4.450	6.720	O	-7.722	4.484	6.648	Ti	-3.166	5.932	3.380
Ti	-3.223	4.449	6.720	O	-3.204	5.935	5.259	O	-5.254	4.477	6.662
O	-1.183	4.444	6.739	Ti	3.358	2.966	3.392	Ti	3.281	1.484	6.751
O	3.299	2.967	5.261	O	1.255	1.487	6.723	O	5.328	1.484	6.719
Ti	-9.676	2.969	3.386	Ti	-9.758	1.485	6.731	O	-9.764	2.967	5.249
O	7.762	1.487	6.717	O	-7.716	1.455	6.687	Ti	-3.151	2.976	3.362
Ti	-3.232	1.479	6.682	O	-3.188	2.971	5.234	O	-5.245	1.442	6.604
O	-1.184	1.484	6.727	Ti	-3.257	-0.000	-3.257	Ti	-3.257	-1.479	-0.009

O	-3.257	-0.000	-1.274	O	-5.240	-1.479	-0.009	O	-1.274	-1.479	-0.009
Ti	3.257	-0.000	-3.257	Ti	3.257	-1.479	-0.009	O	3.257	-0.000	-1.274
O	1.274	-1.479	-0.009	O	5.240	-1.479	-0.009	Ti	-9.771	0.000	-3.257
Ti	-9.771	-1.479	-0.009	O	-9.771	0.000	-1.274	O	7.787	-1.479	-0.009
O	-7.787	-1.479	-0.009	Ti	-3.257	-2.966	-3.257	Ti	-3.257	-4.445	-0.009
O	-3.257	-2.966	-1.274	O	-5.240	-4.445	-0.009	O	-1.274	-4.445	-0.009
Ti	3.257	-2.966	-3.257	Ti	3.257	-4.445	-0.009	O	3.257	-2.966	-1.274
O	1.274	-4.445	-0.009	O	5.240	-4.445	-0.009	Ti	-9.771	-2.966	-3.257
Ti	-9.771	-4.445	-0.009	O	-9.771	-2.966	-1.274	O	7.787	-4.445	-0.009
O	-7.787	-4.445	-0.009	Ti	-3.257	-5.932	-3.257	Ti	-3.257	-7.411	-0.009
O	-3.257	-5.932	-1.274	O	-5.240	-7.411	-0.009	O	-1.274	-7.411	-0.009
Ti	3.257	-5.932	-3.257	Ti	3.257	-7.411	-0.009	O	3.257	-5.932	-1.274
O	1.274	-7.411	-0.009	O	5.240	-7.411	-0.009	Ti	-9.771	-5.932	-3.257
Ti	-9.771	-7.411	-0.009	O	-9.771	-5.932	-1.274	O	7.787	-7.411	-0.009
O	-7.787	-7.411	-0.009	Ti	-3.257	-8.898	-3.257	Ti	-3.257	-10.377	-0.009
O	-3.257	-8.898	-1.274	O	-5.240	-10.377	-0.009	O	-1.274	-10.377	-0.009
Ti	3.257	-8.898	-3.257	Ti	3.257	-10.377	-0.009	O	3.257	-8.898	-1.274
O	1.274	-10.377	-0.009	O	5.240	-10.377	-0.009	Ti	-9.771	-8.898	-3.257
Ti	-9.771	-10.377	-0.009	O	-9.771	-8.898	-1.274	O	7.787	-10.377	-0.009
O	-7.787	-10.377	-0.009	Ti	-3.257	8.898	-3.257	Ti	-3.257	7.419	-0.009
O	-3.257	8.898	-1.274	O	-5.240	7.419	-0.009	O	-1.274	7.419	-0.009
Ti	3.257	8.898	-3.257	Ti	3.257	7.419	-0.009	O	3.257	8.898	-1.274
O	1.274	7.419	-0.009	O	5.240	7.419	-0.009	Ti	-9.771	8.898	-3.257
Ti	-9.771	7.419	-0.009	O	-9.771	8.898	-1.274	O	7.787	7.419	-0.009
O	-7.787	7.419	-0.009	Ti	-3.257	5.932	-3.257	Ti	-3.257	4.453	-0.009
O	-3.257	5.932	-1.274	O	-5.240	4.453	-0.009	O	-1.274	4.453	-0.009
Ti	3.257	5.932	-3.257	Ti	3.257	4.453	-0.009	O	3.257	5.932	-1.274
O	1.274	4.453	-0.009	O	5.240	4.453	-0.009	Ti	-9.771	5.932	-3.257
Ti	-9.771	4.453	-0.009	O	-9.771	5.932	-1.274	O	7.787	4.453	-0.009
O	-7.787	4.453	-0.009	Ti	-3.257	2.966	-3.257	Ti	-3.257	1.487	-0.009
O	-3.257	2.966	-1.274	O	-5.240	1.487	-0.009	O	-1.274	1.487	-0.009

Ti	3.257	2.966	-3.257	Ti	3.257	1.487	-0.009	O	3.257	2.966	-1.274
O	1.274	1.487	-0.009	O	5.240	1.487	-0.009	Ti	-9.771	2.966	-3.257
Ti	-9.771	1.487	-0.009	O	-9.771	2.966	-1.274	O	7.787	1.487	-0.009
O	-7.787	1.487	-0.009	Ti	-6.514	0.000	-6.514	Ti	-6.514	-1.479	-3.266
O	-6.514	0.000	-4.530	O	-6.514	-0.000	-2.001	O	-8.497	-1.479	-3.266
O	-4.530	-1.479	-3.266	Ti	-0.000	-0.000	-6.514	Ti	-0.000	-1.479	-3.266
O	-0.000	-0.000	-4.530	O	-0.000	-0.000	-2.001	O	-1.983	-1.479	-3.266
O	1.983	-1.479	-3.266	Ti	6.514	-0.000	-6.514	Ti	6.514	-1.479	-3.266
O	6.514	-0.000	-4.530	O	6.514	-0.000	-2.001	O	4.530	-1.479	-3.266
O	8.497	-1.479	-3.266	Ti	-6.514	-2.966	-6.514	Ti	-6.514	-4.445	-3.266
O	-6.514	-2.966	-4.530	O	-6.514	-2.966	-2.001	O	-8.497	-4.445	-3.266
O	-4.530	-4.445	-3.266	Ti	-0.000	-2.966	-6.514	Ti	-0.000	-4.445	-3.266
O	-0.000	-2.966	-4.530	O	-0.000	-2.966	-2.001	O	-1.983	-4.445	-3.266
O	1.983	-4.445	-3.266	Ti	6.514	-2.966	-6.514	Ti	6.514	-4.445	-3.266
O	6.514	-2.966	-4.530	O	6.514	-2.966	-2.001	O	4.530	-4.445	-3.266
O	8.497	-4.445	-3.266	Ti	-6.514	-5.932	-6.514	Ti	-6.514	-7.411	-3.266
O	-6.514	-5.932	-4.530	O	-6.514	-5.932	-2.001	O	-8.497	-7.411	-3.266
O	-4.530	-7.411	-3.266	Ti	-0.000	-5.932	-6.514	Ti	-0.000	-7.411	-3.266
O	-0.000	-5.932	-4.530	O	-0.000	-5.932	-2.001	O	-1.983	-7.411	-3.266
O	1.983	-7.411	-3.266	Ti	6.514	-5.932	-6.514	Ti	6.514	-7.411	-3.266
O	6.514	-5.932	-4.530	O	6.514	-5.932	-2.001	O	4.530	-7.411	-3.266
O	8.497	-7.411	-3.266	Ti	-6.514	-8.898	-6.514	Ti	-6.514	-10.377	-3.266
O	-6.514	-8.898	-4.530	O	-6.514	-8.898	-2.001	O	-8.497	-10.377	-3.266
O	-4.530	-10.377	-3.266	Ti	-0.000	-8.898	-6.514	Ti	-0.000	-10.377	-3.266
O	-0.000	-8.898	-4.530	O	-0.000	-8.898	-2.001	O	-1.983	-10.377	-3.266
O	1.983	-10.377	-3.266	Ti	6.514	-8.898	-6.514	Ti	6.514	-10.377	-3.266
O	6.514	-8.898	-4.530	O	6.514	-8.898	-2.001	O	4.530	-10.377	-3.266
O	8.497	-10.377	-3.266	Ti	-6.514	8.898	-6.514	Ti	-6.514	7.419	-3.266
O	-6.514	8.898	-4.530	O	-6.514	8.898	-2.001	O	-8.497	7.419	-3.266
O	-4.530	7.419	-3.266	Ti	0.000	8.898	-6.514	Ti	0.000	7.419	-3.266
O	0.000	8.898	-4.530	O	0.000	8.898	-2.001	O	-1.983	7.419	-3.266

O	1.983	7.419	-3.266	Ti	6.514	8.898	-6.514	Ti	6.514	7.419	-3.266
O	6.514	8.898	-4.530	O	6.514	8.898	-2.001	O	4.530	7.419	-3.266
O	8.497	7.419	-3.266	Ti	-6.514	5.932	-6.514	Ti	-6.514	4.453	-3.266
O	-6.514	5.932	-4.530	O	-6.514	5.932	-2.001	O	-8.497	4.453	-3.266
O	-4.530	4.453	-3.266	Ti	-0.000	5.932	-6.514	Ti	0.000	4.453	-3.266
O	0.000	5.932	-4.530	O	0.000	5.932	-2.001	O	-1.983	4.453	-3.266
O	1.983	4.453	-3.266	Ti	6.514	5.932	-6.514	Ti	6.514	4.453	-3.266
O	6.514	5.932	-4.530	O	6.514	5.932	-2.001	O	4.530	4.453	-3.266
O	8.497	4.453	-3.266	Ti	-6.514	2.966	-6.514	Ti	-6.514	1.487	-3.266
O	-6.514	2.966	-4.530	O	-6.514	2.966	-2.001	O	-8.497	1.487	-3.266
O	-4.530	1.487	-3.266	Ti	-0.000	2.966	-6.514	Ti	-0.000	1.487	-3.266
O	-0.000	2.966	-4.530	O	-0.000	2.966	-2.001	O	-1.983	1.487	-3.266
O	1.983	1.487	-3.266	Ti	6.514	2.966	-6.514	Ti	6.514	1.487	-3.266
O	6.514	2.966	-4.530	O	6.514	2.966	-2.001	O	4.530	1.487	-3.266
O	8.497	1.487	-3.266	Ti	-9.771	-1.479	-6.523	O	-9.771	0.000	-7.787
O	-9.771	0.000	-5.258	O	7.787	-1.479	-6.523	O	-7.787	-1.479	-6.523
Ti	-3.257	-1.479	-6.523	O	-3.257	0.000	-7.787	O	-3.257	-0.000	-5.258
O	-5.240	-1.479	-6.523	O	-1.274	-1.479	-6.523	Ti	3.257	-1.479	-6.523
O	3.257	-0.000	-7.787	O	3.257	-0.000	-5.258	O	1.274	-1.479	-6.523
O	5.240	-1.479	-6.523	Ti	-9.771	-4.445	-6.523	O	-9.771	-2.966	-7.787
O	-9.771	-2.966	-5.258	O	7.787	-4.445	-6.523	O	-7.787	-4.445	-6.523
Ti	-3.257	-4.445	-6.523	O	-3.257	-2.966	-7.787	O	-3.257	-2.966	-5.258
O	-5.240	-4.445	-6.523	O	-1.274	-4.445	-6.523	Ti	3.257	-4.445	-6.523
O	3.257	-2.966	-7.787	O	3.257	-2.966	-5.258	O	1.274	-4.445	-6.523
O	5.240	-4.445	-6.523	Ti	-9.771	-7.411	-6.523	O	-9.771	-5.932	-7.787
O	-9.771	-5.932	-5.258	O	7.787	-7.411	-6.523	O	-7.787	-7.411	-6.523
Ti	-3.257	-7.411	-6.523	O	-3.257	-5.932	-7.787	O	-3.257	-5.932	-5.258
O	-5.240	-7.411	-6.523	O	-1.274	-7.411	-6.523	Ti	3.257	-7.411	-6.523
O	3.257	-5.932	-7.787	O	3.257	-5.932	-5.258	O	1.274	-7.411	-6.523
O	5.240	-7.411	-6.523	Ti	-9.771	-10.377	-6.523	O	-9.771	-8.898	-7.787
O	-9.771	-8.898	-5.258	O	7.787	-10.377	-6.523	O	-7.787	-10.377	-6.523

Ti	-3.257	-10.377	-6.523	O	-3.257	-8.898	-7.787	O	-3.257	-8.898	-5.258
O	-5.240	-10.377	-6.523	O	-1.274	-10.377	-6.523	Ti	3.257	-10.377	-6.523
O	3.257	-8.898	-7.787	O	3.257	-8.898	-5.258	O	1.274	-10.377	-6.523
O	5.240	-10.377	-6.523	Ti	-9.771	7.419	-6.523	O	-9.771	8.898	-7.787
O	-9.771	8.898	-5.258	O	7.787	7.419	-6.523	O	-7.787	7.419	-6.523
Ti	-3.257	7.419	-6.523	O	-3.257	8.898	-7.787	O	-3.257	8.898	-5.258
O	-5.240	7.419	-6.523	O	-1.274	7.419	-6.523	Ti	3.257	7.419	-6.523
O	3.257	8.898	-7.787	O	3.257	8.898	-5.258	O	1.274	7.419	-6.523
O	5.240	7.419	-6.523	Ti	-9.771	4.453	-6.523	O	-9.771	5.932	-7.787
O	-9.771	5.932	-5.258	O	7.787	4.453	-6.523	O	-7.787	4.453	-6.523
Ti	-3.257	4.453	-6.523	O	-3.257	5.932	-7.787	O	-3.257	5.932	-5.258
O	-5.240	4.453	-6.523	O	-1.274	4.453	-6.523	Ti	3.257	4.453	-6.523
O	3.257	5.932	-7.787	O	3.257	5.932	-5.258	O	1.274	4.453	-6.523
O	5.240	4.453	-6.523	Ti	-9.771	1.487	-6.523	O	-9.771	2.966	-7.787
O	-9.771	2.966	-5.258	O	7.787	1.487	-6.523	O	-7.787	1.487	-6.523
Ti	-3.257	1.487	-6.523	O	-3.257	2.966	-7.787	O	-3.257	2.966	-5.258
O	-5.240	1.487	-6.523	O	-1.274	1.487	-6.523	Ti	3.257	1.487	-6.523
O	3.257	2.966	-7.787	O	3.257	2.966	-5.258	O	1.274	1.487	-6.523
O	5.240	1.487	-6.523								

Table S2: Pyr monomer on rutile TiO_2 (110) surface

C	-7.287	-0.178	9.917	C	-7.874	-1.428	9.928	C	-7.107	-2.579	10.172
C	-5.746	-2.453	10.430	C	-5.900	-0.052	10.165	C	-5.209	1.206	10.140
C	-5.869	2.207	9.455	C	-3.809	1.442	10.501	C	-3.352	2.767	10.687
C	-2.000	2.996	10.881	C	-1.115	1.916	10.835	C	-1.637	0.628	10.651
C	-4.843	-3.606	10.630	C	-5.367	-4.895	10.797	C	-4.483	-5.975	10.848
C	-3.128	-5.744	10.673	C	-2.670	-4.419	10.495	C	-1.268	-4.182	10.142
C	-0.604	-5.181	9.459	C	-0.578	-2.923	10.171	C	-0.733	-0.522	10.446
C	0.627	-0.394	10.188	C	1.395	-1.543	9.934	C	0.809	-2.794	9.920
H	-7.883	0.709	9.709	H	-8.936	-1.527	9.710	H	-7.577	-3.556	10.123
H	-4.170	-1.062	10.510	H	-4.059	3.593	10.657	H	-1.629	4.008	11.035
H	-0.046	2.078	10.945	H	-6.437	-5.059	10.891	H	-4.855	-6.988	10.990
H	-2.421	-6.571	10.646	H	-2.309	-1.916	10.515	H	1.095	0.584	10.143
H	2.455	-1.442	9.713	H	1.405	-3.679	9.706	N	-5.198	-1.201	10.417
N	-2.964	0.384	10.557	N	-3.515	-3.361	10.550	N	-1.281	-1.775	10.427
N	-0.024	-5.941	8.759	N	-6.441	2.972	8.754	O	3.292	-0.006	7.825
O	-9.746	-0.003	7.811	O	-3.244	-0.002	7.780	O	-3.212	-2.966	7.781
O	3.297	-2.957	7.818	O	-9.735	-2.952	7.822	O	3.263	-5.925	7.814
O	-9.733	-5.922	7.835	O	-3.193	-5.920	7.784	O	3.294	-8.894	7.822
O	-9.732	-8.892	7.830	O	-3.215	-8.889	7.821	O	3.295	8.896	7.826
O	-9.734	8.901	7.826	O	-3.220	8.896	7.830	O	3.292	5.929	7.831
O	-9.730	5.931	7.821	O	-3.227	5.917	7.827	O	3.291	2.962	7.834
O	-9.717	2.965	7.810	O	-3.260	2.953	7.788	Ti	6.543	-0.001	6.372
Ti	-6.467	0.010	6.346	Ti	0.036	-0.007	6.363	Ti	6.540	-2.963	6.373
Ti	-6.497	-2.955	6.360	Ti	0.008	-2.973	6.352	Ti	6.564	-5.929	6.375
Ti	-6.469	-5.922	6.371	Ti	6.548	-8.899	6.377	Ti	-6.484	-8.892	6.371
Ti	0.018	-8.911	6.353	Ti	6.548	8.899	6.378	Ti	-6.481	8.902	6.359
Ti	0.036	8.894	6.361	Ti	6.545	5.938	6.377	Ti	-6.466	5.948	6.352
Ti	0.035	5.927	6.372	Ti	6.524	2.968	6.375	Ti	-6.540	2.997	6.618
Ti	0.080	-5.959	6.622	Ti	0.014	2.960	6.373	Ti	0.119	-1.516	3.139

O	0.026	0.007	1.999	O	0.018	0.000	4.556	O	-1.934	-1.483	3.245
O	1.991	-1.481	3.272	Ti	6.635	-1.482	3.188	O	6.534	0.002	2.006
O	6.536	0.003	4.561	O	4.578	-1.482	3.266	O	8.493	-1.486	3.272
Ti	-6.391	-1.448	3.138	O	-6.495	0.024	2.001	O	-6.492	-0.014	4.541
O	-8.456	-1.484	3.266	O	-4.527	-1.477	3.254	Ti	0.115	-4.498	3.271
O	0.026	-2.985	2.002	O	0.022	-2.942	4.546	O	-1.942	-4.442	3.271
O	1.993	-4.441	3.287	Ti	6.632	-4.447	3.188	O	6.536	-2.966	2.005
O	6.533	-2.968	4.562	O	4.580	-4.446	3.261	O	8.496	-4.451	3.277
Ti	-6.388	-4.434	3.200	O	-6.497	-2.969	1.998	O	-6.488	-2.963	4.554
O	-8.456	-4.448	3.271	O	-4.531	-4.446	3.262	Ti	0.118	-7.359	3.270
O	0.024	-5.929	2.020	O	0.034	-5.927	4.590	O	-1.942	-7.414	3.275
O	1.993	-7.415	3.291	Ti	6.630	-7.412	3.191	O	6.536	-5.931	2.006
O	6.535	-5.926	4.565	O	4.580	-7.411	3.267	O	8.496	-7.410	3.285
Ti	-6.391	-7.411	3.174	O	-6.497	-5.924	2.006	O	-6.490	-5.927	4.562
O	-8.455	-7.410	3.272	O	-4.532	-7.412	3.266	Ti	0.118	-10.347	3.139
O	0.024	-8.877	2.004	O	0.016	-8.918	4.549	O	-1.939	-10.380	3.265
O	1.989	-10.381	3.276	Ti	6.632	-10.380	3.190	O	6.537	-8.895	2.008
O	6.533	-8.895	4.566	O	4.578	-10.382	3.269	O	8.496	-10.378	3.284
Ti	-6.385	-10.390	3.200	O	-6.495	-8.898	2.007	O	-6.490	-8.890	4.562
O	-8.455	-10.377	3.274	O	-4.530	-10.382	3.279	Ti	0.123	7.426	3.202
O	0.023	8.893	2.001	O	0.021	8.897	4.558	O	-1.937	7.416	3.270
O	1.985	7.412	3.285	Ti	6.635	7.417	3.191	O	6.534	8.900	2.008
O	6.534	8.898	4.566	O	4.575	7.413	3.272	O	8.494	7.422	3.276
Ti	-6.396	7.383	3.137	O	-6.494	8.905	2.000	O	-6.492	8.899	4.555
O	-8.454	7.416	3.267	O	-4.525	7.418	3.273	Ti	0.121	4.450	3.175
O	0.024	5.939	2.007	O	0.019	5.924	4.564	O	-1.934	4.458	3.257
O	1.986	4.450	3.280	Ti	6.631	4.453	3.189	O	6.533	5.935	2.007
O	6.535	5.933	4.565	O	4.575	4.450	3.273	O	8.493	4.455	3.272
Ti	-6.398	4.397	3.272	O	-6.493	5.912	2.004	O	-6.488	5.960	4.549
O	-8.460	4.457	3.283	O	-4.522	4.459	3.287	Ti	0.124	1.472	3.201
O	0.025	2.965	2.006	O	0.017	2.970	4.563	O	-1.933	1.488	3.252

O	1.986	1.486	3.283	Ti	6.632	1.486	3.187	O	6.533	2.972	2.006
O	6.533	2.970	4.564	O	4.576	1.487	3.269	O	8.492	1.486	3.269
Ti	-6.389	1.537	3.266	O	-6.492	2.973	2.019	O	-6.490	2.969	4.586
O	-8.461	1.485	3.277	O	-4.520	1.485	3.280	Ti	3.360	-0.006	3.380
Ti	3.278	-1.483	6.716	O	3.304	0.005	5.253	O	1.265	-1.470	6.684
O	5.331	-1.481	6.717	Ti	-9.666	0.003	3.369	Ti	-9.739	-1.480	6.709
O	-9.760	-0.001	5.242	O	7.765	-1.485	6.706	O	-7.717	-1.492	6.676
Ti	-3.153	0.008	3.354	Ti	-3.231	-1.489	6.703	O	-3.194	-0.008	5.227
O	-5.273	-1.488	6.732	O	-1.179	-1.479	6.739	Ti	3.350	-2.969	3.373
Ti	3.303	-4.445	6.733	O	3.312	-2.962	5.251	O	1.265	-4.414	6.693
O	5.335	-4.450	6.732	Ti	-9.669	-2.967	3.377	Ti	-9.733	-4.445	6.748
O	-9.743	-2.972	5.249	O	7.772	-4.445	6.712	O	-7.697	-4.448	6.737
Ti	-3.155	-2.956	3.354	Ti	-3.225	-4.449	6.688	O	-3.245	-2.943	5.227
O	-5.260	-4.447	6.714	O	-1.202	-4.417	6.622	Ti	3.359	-5.929	3.385
Ti	3.314	-7.416	6.743	O	3.318	-5.919	5.254	O	1.278	-7.455	6.636
O	5.337	-7.408	6.728	Ti	-9.670	-5.930	3.392	Ti	-9.726	-7.410	6.755
O	-9.726	-5.922	5.263	O	7.776	-7.410	6.707	O	-7.694	-7.406	6.726
Ti	-3.158	-5.929	3.369	Ti	-3.228	-7.422	6.722	O	-3.251	-5.927	5.232
O	-5.258	-7.408	6.723	O	-1.192	-7.442	6.657	Ti	3.351	-8.894	3.387
Ti	3.283	-10.383	6.748	O	3.319	-8.900	5.254	O	1.261	-10.391	6.698
O	5.336	-10.380	6.724	Ti	-9.669	-8.894	3.392	Ti	-9.734	-10.378	6.752
O	-9.725	-8.889	5.260	O	7.775	-10.377	6.703	O	-7.695	-10.373	6.716
Ti	-3.152	-8.899	3.380	Ti	-3.230	-10.389	6.751	O	-3.234	-8.896	5.249
O	-5.255	-10.374	6.709	O	-1.184	-10.391	6.712	Ti	3.358	8.904	3.389
Ti	3.289	7.414	6.751	O	3.304	8.895	5.259	O	1.260	7.405	6.703
O	5.332	7.413	6.719	Ti	-9.666	8.903	3.389	Ti	-9.730	7.419	6.746
O	-9.727	8.900	5.258	O	7.770	7.417	6.714	O	-7.695	7.426	6.711
Ti	-3.152	8.890	3.393	Ti	-3.214	7.405	6.754	O	-3.210	8.899	5.261
O	-5.251	7.427	6.700	O	-1.180	7.406	6.727	Ti	3.358	5.934	3.391
Ti	3.277	4.450	6.753	O	3.300	5.923	5.261	O	1.254	4.443	6.717
O	5.328	4.452	6.722	Ti	-9.673	5.937	3.385	Ti	-9.768	4.457	6.739

O	-9.762	5.945	5.252	O	7.762	4.449	6.720	O	-7.726	4.488	6.631
Ti	-3.164	5.932	3.381	Ti	-3.227	4.444	6.723	O	-3.204	5.940	5.257
O	-5.257	4.476	6.658	O	-1.184	4.444	6.737	Ti	3.357	2.967	3.391
Ti	3.277	1.485	6.750	O	3.298	2.966	5.262	O	1.253	1.486	6.725
O	5.327	1.484	6.720	Ti	-9.676	2.970	3.385	Ti	-9.762	1.485	6.728
O	-9.766	2.966	5.247	O	7.761	1.487	6.719	O	-7.718	1.453	6.681
Ti	-3.150	2.974	3.366	Ti	-3.236	1.474	6.690	O	-3.190	2.975	5.236
O	-5.250	1.448	6.617	O	-1.185	1.484	6.729	O	-3.257	0.000	1.256
O	3.257	0.000	1.256	O	-9.771	0.000	1.256	O	-3.257	-2.966	1.256
O	3.257	-2.966	1.256	O	-9.771	-2.966	1.256	O	-3.257	-5.932	1.256
O	3.257	-5.932	1.256	O	-9.771	-5.932	1.256	O	-3.257	-8.898	1.256
O	3.257	-8.898	1.256	O	-9.771	-8.898	1.256	O	-3.257	8.898	1.256
O	3.257	8.898	1.256	O	-9.771	8.898	1.256	O	-3.257	5.932	1.256
O	3.257	5.932	1.256	O	-9.771	5.932	1.256	O	-3.257	2.966	1.256
O	3.257	2.966	1.256	O	-9.771	2.966	1.256	Ti	0.000	0.000	0.000
Ti	6.514	0.000	0.000	Ti	-6.514	0.000	0.000	Ti	-0.000	-2.966	0.000
Ti	6.514	-2.966	0.000	Ti	-6.514	-2.966	0.000	Ti	-0.000	-5.932	0.000
Ti	6.514	-5.932	0.000	Ti	-6.514	-5.932	0.000	Ti	-0.000	-8.898	0.000
Ti	6.514	-8.898	0.000	Ti	-6.514	-8.898	0.000	Ti	0.000	8.898	0.000
Ti	6.514	8.898	0.000	Ti	-6.514	8.898	0.000	Ti	0.000	5.932	0.000
Ti	6.514	5.932	0.000	Ti	-6.514	5.932	0.000	Ti	0.000	2.966	0.000
Ti	6.514	2.966	0.000	Ti	-6.514	2.966	0.000	Ti	-3.257	-1.479	-0.009
O	-3.257	-0.000	-1.274	O	-5.240	-1.479	-0.009	O	-1.274	-1.479	-0.009
Ti	3.257	-1.479	-0.009	O	3.257	-0.000	-1.274	O	1.274	-1.479	-0.009
O	5.240	-1.479	-0.009	Ti	-9.771	-1.479	-0.009	O	-9.771	0.000	-1.274
O	7.787	-1.479	-0.009	O	-7.787	-1.479	-0.009	Ti	-3.257	-4.445	-0.009
O	-3.257	-2.966	-1.274	O	-5.240	-4.445	-0.009	O	-1.274	-4.445	-0.009
Ti	3.257	-4.445	-0.009	O	3.257	-2.966	-1.274	O	1.274	-4.445	-0.009
O	5.240	-4.445	-0.009	Ti	-9.771	-4.445	-0.009	O	-9.771	-2.966	-1.274
O	7.787	-4.445	-0.009	O	-7.787	-4.445	-0.009	Ti	-3.257	-7.411	-0.009
O	-3.257	-5.932	-1.274	O	-5.240	-7.411	-0.009	O	-1.274	-7.411	-0.009

Ti	3.257	-7.411	-0.009	O	3.257	-5.932	-1.274	O	1.274	-7.411	-0.009
O	5.240	-7.411	-0.009	Ti	-9.771	-7.411	-0.009	O	-9.771	-5.932	-1.274
O	7.787	-7.411	-0.009	O	-7.787	-7.411	-0.009	Ti	-3.257	-10.377	-0.009
O	-3.257	-8.898	-1.274	O	-5.240	-10.377	-0.009	O	-1.274	-10.377	-0.009
Ti	3.257	-10.377	-0.009	O	3.257	-8.898	-1.274	O	1.274	-10.377	-0.009
O	5.240	-10.377	-0.009	Ti	-9.771	-10.377	-0.009	O	-9.771	-8.898	-1.274
O	7.787	-10.377	-0.009	O	-7.787	-10.377	-0.009	Ti	-3.257	7.419	-0.009
O	-3.257	8.898	-1.274	O	-5.240	7.419	-0.009	O	-1.274	7.419	-0.009
Ti	3.257	7.419	-0.009	O	3.257	8.898	-1.274	O	1.274	7.419	-0.009
O	5.240	7.419	-0.009	Ti	-9.771	7.419	-0.009	O	-9.771	8.898	-1.274
O	7.787	7.419	-0.009	O	-7.787	7.419	-0.009	Ti	-3.257	4.453	-0.009
O	-3.257	5.932	-1.274	O	-5.240	4.453	-0.009	O	-1.274	4.453	-0.009
Ti	3.257	4.453	-0.009	O	3.257	5.932	-1.274	O	1.274	4.453	-0.009
O	5.240	4.453	-0.009	Ti	-9.771	4.453	-0.009	O	-9.771	5.932	-1.274
O	7.787	4.453	-0.009	O	-7.787	4.453	-0.009	Ti	-3.257	1.487	-0.009
O	-3.257	2.966	-1.274	O	-5.240	1.487	-0.009	O	-1.274	1.487	-0.009
Ti	3.257	1.487	-0.009	O	3.257	2.966	-1.274	O	1.274	1.487	-0.009
O	5.240	1.487	-0.009	Ti	-9.771	1.487	-0.009	O	-9.771	2.966	-1.274
O	7.787	1.487	-0.009	O	-7.787	1.487	-0.009	Ti	-3.257	-0.000	-3.257
Ti	3.257	-0.000	-3.257	Ti	-9.771	0.000	-3.257	Ti	-3.257	-2.966	-3.257
Ti	3.257	-2.966	-3.257	Ti	-9.771	-2.966	-3.257	Ti	-3.257	-5.932	-3.257
Ti	3.257	-5.932	-3.257	Ti	-9.771	-5.932	-3.257	Ti	-3.257	-8.898	-3.257
Ti	3.257	-8.898	-3.257	Ti	-9.771	-8.898	-3.257	Ti	-3.257	8.898	-3.257
Ti	3.257	8.898	-3.257	Ti	-9.771	8.898	-3.257	Ti	-3.257	5.932	-3.257
Ti	3.257	5.932	-3.257	Ti	-9.771	5.932	-3.257	Ti	-3.257	2.966	-3.257
Ti	3.257	2.966	-3.257	Ti	-9.771	2.966	-3.257	Ti	-6.514	0.000	-6.514
Ti	-6.514	-1.479	-3.266	O	-6.514	0.000	-4.530	O	-6.514	-0.000	-2.001
O	-8.497	-1.479	-3.266	O	-4.530	-1.479	-3.266	Ti	-0.000	-0.000	-6.514
Ti	-0.000	-1.479	-3.266	O	-0.000	-0.000	-4.530	O	-0.000	-0.000	-2.001
O	-1.983	-1.479	-3.266	O	1.983	-1.479	-3.266	Ti	6.514	-0.000	-6.514
Ti	6.514	-1.479	-3.266	O	6.514	-0.000	-4.530	O	6.514	-0.000	-2.001

O	4.530	-1.479	-3.266	O	8.497	-1.479	-3.266	Ti	-6.514	-2.966	-6.514
Ti	-6.514	-4.445	-3.266	O	-6.514	-2.966	-4.530	O	-6.514	-2.966	-2.001
O	-8.497	-4.445	-3.266	O	-4.530	-4.445	-3.266	Ti	-0.000	-2.966	-6.514
Ti	-0.000	-4.445	-3.266	O	-0.000	-2.966	-4.530	O	-0.000	-2.966	-2.001
O	-1.983	-4.445	-3.266	O	1.983	-4.445	-3.266	Ti	6.514	-2.966	-6.514
Ti	6.514	-4.445	-3.266	O	6.514	-2.966	-4.530	O	6.514	-2.966	-2.001
O	4.530	-4.445	-3.266	O	8.497	-4.445	-3.266	Ti	-6.514	-5.932	-6.514
Ti	-6.514	-7.411	-3.266	O	-6.514	-5.932	-4.530	O	-6.514	-5.932	-2.001
O	-8.497	-7.411	-3.266	O	-4.530	-7.411	-3.266	Ti	-0.000	-5.932	-6.514
Ti	-0.000	-7.411	-3.266	O	-0.000	-5.932	-4.530	O	-0.000	-5.932	-2.001
O	-1.983	-7.411	-3.266	O	1.983	-7.411	-3.266	Ti	6.514	-5.932	-6.514
Ti	6.514	-7.411	-3.266	O	6.514	-5.932	-4.530	O	6.514	-5.932	-2.001
O	4.530	-7.411	-3.266	O	8.497	-7.411	-3.266	Ti	-6.514	-8.898	-6.514
Ti	-6.514	-10.377	-3.266	O	-6.514	-8.898	-4.530	O	-6.514	-8.898	-2.001
O	-8.497	-10.377	-3.266	O	-4.530	-10.377	-3.266	Ti	-0.000	-8.898	-6.514
Ti	-0.000	-10.377	-3.266	O	-0.000	-8.898	-4.530	O	-0.000	-8.898	-2.001
O	-1.983	-10.377	-3.266	O	1.983	-10.377	-3.266	Ti	6.514	-8.898	-6.514
Ti	6.514	-10.377	-3.266	O	6.514	-8.898	-4.530	O	6.514	-8.898	-2.001
O	4.530	-10.377	-3.266	O	8.497	-10.377	-3.266	Ti	-6.514	8.898	-6.514
Ti	-6.514	7.419	-3.266	O	-6.514	8.898	-4.530	O	-6.514	8.898	-2.001
O	-8.497	7.419	-3.266	O	-4.530	7.419	-3.266	Ti	0.000	8.898	-6.514
Ti	0.000	7.419	-3.266	O	0.000	8.898	-4.530	O	0.000	8.898	-2.001
O	-1.983	7.419	-3.266	O	1.983	7.419	-3.266	Ti	6.514	8.898	-6.514
Ti	6.514	7.419	-3.266	O	6.514	8.898	-4.530	O	6.514	8.898	-2.001
O	4.530	7.419	-3.266	O	8.497	7.419	-3.266	Ti	-6.514	5.932	-6.514
Ti	-6.514	4.453	-3.266	O	-6.514	5.932	-4.530	O	-6.514	5.932	-2.001
O	-8.497	4.453	-3.266	O	-4.530	4.453	-3.266	Ti	-0.000	5.932	-6.514
Ti	0.000	4.453	-3.266	O	0.000	5.932	-4.530	O	0.000	5.932	-2.001
O	-1.983	4.453	-3.266	O	1.983	4.453	-3.266	Ti	6.514	5.932	-6.514
Ti	6.514	4.453	-3.266	O	6.514	5.932	-4.530	O	6.514	5.932	-2.001
O	4.530	4.453	-3.266	O	8.497	4.453	-3.266	Ti	-6.514	2.966	-6.514

Ti	-6.514	1.487	-3.266	O	-6.514	2.966	-4.530	O	-6.514	2.966	-2.001
O	-8.497	1.487	-3.266	O	-4.530	1.487	-3.266	Ti	-0.000	2.966	-6.514
Ti	-0.000	1.487	-3.266	O	-0.000	2.966	-4.530	O	-0.000	2.966	-2.001
O	-1.983	1.487	-3.266	O	1.983	1.487	-3.266	Ti	6.514	2.966	-6.514
Ti	6.514	1.487	-3.266	O	6.514	2.966	-4.530	O	6.514	2.966	-2.001
O	4.530	1.487	-3.266	O	8.497	1.487	-3.266	Ti	-9.771	-1.479	-6.523
O	-9.771	0.000	-7.787	O	-9.771	0.000	-5.258	O	7.787	-1.479	-6.523
O	-7.787	-1.479	-6.523	Ti	-3.257	-1.479	-6.523	O	-3.257	0.000	-7.787
O	-3.257	-0.000	-5.258	O	-5.240	-1.479	-6.523	O	-1.274	-1.479	-6.523
Ti	3.257	-1.479	-6.523	O	3.257	-0.000	-7.787	O	3.257	-0.000	-5.258
O	1.274	-1.479	-6.523	O	5.240	-1.479	-6.523	Ti	-9.771	-4.445	-6.523
O	-9.771	-2.966	-7.787	O	-9.771	-2.966	-5.258	O	7.787	-4.445	-6.523
O	-7.787	-4.445	-6.523	Ti	-3.257	-4.445	-6.523	O	-3.257	-2.966	-7.787
O	-3.257	-2.966	-5.258	O	-5.240	-4.445	-6.523	O	-1.274	-4.445	-6.523
Ti	3.257	-4.445	-6.523	O	3.257	-2.966	-7.787	O	3.257	-2.966	-5.258
O	1.274	-4.445	-6.523	O	5.240	-4.445	-6.523	Ti	-9.771	-7.411	-6.523
O	-9.771	-5.932	-7.787	O	-9.771	-5.932	-5.258	O	7.787	-7.411	-6.523
O	-7.787	-7.411	-6.523	Ti	-3.257	-7.411	-6.523	O	-3.257	-5.932	-7.787
O	-3.257	-5.932	-5.258	O	-5.240	-7.411	-6.523	O	-1.274	-7.411	-6.523
Ti	3.257	-7.411	-6.523	O	3.257	-5.932	-7.787	O	3.257	-5.932	-5.258
O	1.274	-7.411	-6.523	O	5.240	-7.411	-6.523	Ti	-9.771	-10.377	-6.523
O	-9.771	-8.898	-7.787	O	-9.771	-8.898	-5.258	O	7.787	-10.377	-6.523
O	-7.787	-10.377	-6.523	Ti	-3.257	-10.377	-6.523	O	-3.257	-8.898	-7.787
O	-3.257	-8.898	-5.258	O	-5.240	-10.377	-6.523	O	-1.274	-10.377	-6.523
Ti	3.257	-10.377	-6.523	O	3.257	-8.898	-7.787	O	3.257	-8.898	-5.258
O	1.274	-10.377	-6.523	O	5.240	-10.377	-6.523	Ti	-9.771	7.419	-6.523
O	-9.771	8.898	-7.787	O	-9.771	8.898	-5.258	O	7.787	7.419	-6.523
O	-7.787	7.419	-6.523	Ti	-3.257	7.419	-6.523	O	-3.257	8.898	-7.787
O	-3.257	8.898	-5.258	O	-5.240	7.419	-6.523	O	-1.274	7.419	-6.523
Ti	3.257	7.419	-6.523	O	3.257	8.898	-7.787	O	3.257	8.898	-5.258
O	1.274	7.419	-6.523	O	5.240	7.419	-6.523	Ti	-9.771	4.453	-6.523

O	-9.771	5.932	-7.787	O	-9.771	5.932	-5.258	O	7.787	4.453	-6.523
O	-7.787	4.453	-6.523	Ti	-3.257	4.453	-6.523	O	-3.257	5.932	-7.787
O	-3.257	5.932	-5.258	O	-5.240	4.453	-6.523	O	-1.274	4.453	-6.523
Ti	3.257	4.453	-6.523	O	3.257	5.932	-7.787	O	3.257	5.932	-5.258
O	1.274	4.453	-6.523	O	5.240	4.453	-6.523	Ti	-9.771	1.487	-6.523
O	-9.771	2.966	-7.787	O	-9.771	2.966	-5.258	O	7.787	1.487	-6.523
O	-7.787	1.487	-6.523	Ti	-3.257	1.487	-6.523	O	-3.257	2.966	-7.787
O	-3.257	2.966	-5.258	O	-5.240	1.487	-6.523	O	-1.274	1.487	-6.523
Ti	3.257	1.487	-6.523	O	3.257	2.966	-7.787	O	3.257	2.966	-5.258
O	1.274	1.487	-6.523	O	5.240	1.487	-6.523				

Table S3: CoPyr monolayer on rutile TiO_2 (110) surface

Co	-9.772	13.343	10.414	C	-10.411	16.209	10.460	C	-10.028	17.560	10.653
C	-8.701	17.893	10.845	C	-7.734	16.883	10.799	C	-8.151	15.567	10.624
C	-9.516	9.127	10.654	C	-9.132	10.477	10.463	C	-7.774	10.790	10.094
C	-7.078	9.788	9.434	C	-7.148	12.089	10.117	C	-7.250	14.442	10.421
C	-5.894	14.587	10.167	C	-5.152	13.444	9.866	C	-5.762	12.207	9.849
H	-8.413	18.934	10.983	H	-6.675	17.111	10.886	H	-8.751	8.355	10.611
H	-5.429	15.569	10.138	H	-4.110	13.548	9.595	H	-5.183	11.320	9.597
N	-9.474	15.219	10.536	N	-10.070	11.468	10.536	N	-7.881	13.220	10.375
N	-6.503	9.007	8.758	C	-0.754	14.481	9.848	C	-1.366	13.245	9.874
C	-0.624	12.102	10.175	C	0.733	12.246	10.420	C	0.633	14.598	10.112
C	1.259	15.897	10.087	C	0.563	16.902	9.430	C	1.635	11.120	10.620
C	1.217	9.803	10.790	C	2.183	8.793	10.837	H	-1.333	15.368	9.597
H	-2.411	13.143	9.613	H	-1.093	11.122	10.157	H	2.235	18.331	10.607
H	0.158	9.575	10.871	H	1.895	7.752	10.970	N	1.365	13.467	10.369
N	-0.010	17.687	8.757	Co	-3.257	25.215	10.413	C	-7.267	26.351	9.846
C	-7.878	25.115	9.868	C	-7.137	23.972	10.169	C	-5.780	24.116	10.418
C	-5.880	26.469	10.112	C	-5.255	27.768	10.089	C	-5.950	28.772	9.431
C	-3.897	28.080	10.460	C	-1.219	28.754	10.794	C	-1.636	27.438	10.621
C	-4.879	22.991	10.620	C	-5.296	21.675	10.794	C	-4.330	20.665	10.841
C	-3.002	20.998	10.652	C	-2.618	22.348	10.460	C	-1.260	22.661	10.089
C	-0.564	21.657	9.432	C	-0.634	23.960	10.114	C	-0.735	26.313	10.420
C	0.622	26.456	10.171	C	1.364	25.313	9.872	C	0.753	24.077	9.849
H	-7.846	27.238	9.595	H	-8.922	25.012	9.602	H	-7.604	22.991	10.146
H	-6.355	21.447	10.878	H	-4.618	19.624	10.977	H	-2.237	20.226	10.608
H	1.089	27.437	10.148	H	2.408	25.415	9.608	H	1.332	23.189	9.599
N	-5.148	25.338	10.369	N	-2.959	27.089	10.535	N	-3.556	23.339	10.535
N	-1.367	25.091	10.371	N	0.010	20.874	8.757	C	-3.513	5.702	10.654
C	-2.186	6.036	10.841	H	-4.279	6.474	10.610	H	-1.898	7.077	10.977
H	-0.160	5.254	10.877	N	-6.524	5.828	8.757	O	-9.750	8.911	7.793

O	-3.274	8.902	7.821	O	-9.755	5.933	7.817	O	-3.279	5.925	7.796
Ti	-6.412	8.900	6.572	Ti	0.050	8.910	6.366	Ti	-6.618	5.942	6.570
Ti	-0.053	5.932	6.366	Ti	0.091	7.420	3.172	O	-0.001	8.905	2.003
O	0.008	8.903	4.561	O	-1.957	7.431	3.268	O	1.958	7.418	3.263
Ti	-6.421	7.421	3.354	O	-6.511	8.881	2.021	O	-6.495	8.921	4.595
O	-8.485	7.427	3.288	O	-4.539	7.421	3.291	O	-0.003	5.935	2.003
O	-0.007	5.938	4.561	O	-6.510	5.964	2.021	O	-6.521	5.923	4.594
O	1.216	7.411	6.738	Ti	-9.699	8.904	3.371	Ti	-9.790	7.415	6.724
O	-9.817	8.906	5.241	O	-7.754	7.446	6.622	Ti	-3.187	8.906	3.378
Ti	-3.241	7.414	6.724	O	-3.239	8.909	5.258	O	-5.273	7.393	6.627
O	-1.216	7.433	6.739	Ti	-9.696	5.940	3.380	O	-9.782	5.933	5.255
Ti	-3.180	5.947	3.368	O	-3.201	5.936	5.248	O	-9.788	20.766	7.820
O	-3.236	20.775	7.792	O	-9.793	17.789	7.796	O	-3.241	17.797	7.817
O	-9.777	14.822	7.787	O	-3.255	14.822	7.804	O	-9.764	11.879	7.786
O	-3.260	11.877	7.804	O	-9.769	26.686	7.804	O	-3.263	26.685	7.787
O	-9.774	23.741	7.804	O	-3.250	23.742	7.786	Ti	-6.465	20.774	6.366
Ti	0.102	20.764	6.572	Ti	-6.566	17.796	6.365	Ti	-0.104	17.806	6.569
Ti	-6.497	14.829	6.355	Ti	0.034	14.832	6.325	Ti	-6.553	11.872	6.327
Ti	-0.021	11.876	6.354	Ti	-6.480	26.696	6.326	Ti	0.016	26.693	6.355
Ti	-6.535	23.740	6.354	Ti	-0.040	23.736	6.327	Ti	0.093	19.285	3.353
O	0.003	20.745	2.021	O	0.019	20.785	4.594	O	-1.971	19.291	3.288
O	1.975	19.285	3.290	Ti	-6.422	19.284	3.171	O	-6.515	20.769	2.003
O	-6.506	20.767	4.561	O	-8.471	19.295	3.268	O	-4.556	19.282	3.263
Ti	0.098	16.396	3.207	O	0.004	17.828	2.020	O	-0.008	17.787	4.594
O	-1.967	16.322	3.271	O	1.974	16.325	3.271	Ti	-6.403	16.301	3.189
O	-6.517	17.799	2.003	O	-6.520	17.802	4.561	O	-8.473	16.323	3.261
O	-4.552	16.325	3.264	Ti	0.111	13.392	3.148	O	0.000	14.857	1.994
O	0.001	14.821	4.529	O	-1.962	13.355	3.263	O	1.965	13.358	3.252
Ti	-6.401	13.313	3.150	O	-6.513	14.837	1.996	O	-6.516	14.837	4.549
O	-8.474	13.357	3.257	O	-4.547	13.358	3.259	Ti	0.110	10.403	3.189
O	-0.003	11.868	1.995	O	0.003	11.868	4.548	O	-1.961	10.388	3.269

O	1.961	10.394	3.255	Ti	-6.428	10.309	3.207	O	-6.512	11.852	1.994
O	-6.519	11.886	4.531	O	-8.480	10.388	3.272	O	-4.542	10.396	3.269
Ti	0.111	28.165	3.189	O	-1.959	28.187	3.261	O	1.962	28.189	3.264
Ti	-6.417	28.261	3.207	O	-8.480	28.186	3.271	O	-4.540	28.189	3.271
Ti	0.112	25.177	3.150	O	0.001	26.701	1.996	O	-0.002	26.701	4.549
O	-1.961	25.221	3.257	O	1.967	25.222	3.259	Ti	-6.403	25.256	3.148
O	-6.514	26.722	1.994	O	-6.513	26.685	4.530	O	-8.476	25.220	3.263
O	-4.549	25.222	3.251	Ti	0.087	22.174	3.208	O	0.002	23.716	1.994
O	-0.006	23.750	4.530	O	-1.966	22.252	3.272	O	1.972	22.260	3.269
Ti	-6.403	22.268	3.189	O	-6.517	23.733	1.995	O	-6.511	23.732	4.548
O	-8.475	22.252	3.269	O	-4.553	22.258	3.255	O	1.241	19.257	6.627
Ti	-9.701	20.770	3.378	Ti	-9.755	19.278	6.724	O	-9.753	20.772	5.258
O	-7.730	19.296	6.739	Ti	-3.184	20.768	3.370	Ti	-3.276	19.279	6.724
O	-3.303	20.770	5.241	O	-5.297	19.275	6.737	O	-1.240	19.310	6.622
O	1.239	16.272	6.611	Ti	-9.693	17.811	3.367	Ti	-9.796	16.312	6.692
O	-9.715	17.799	5.248	O	-7.735	16.319	6.730	Ti	-3.181	17.804	3.380
Ti	-3.292	16.308	6.726	O	-3.267	17.797	5.254	O	-5.300	16.331	6.734
O	-1.237	16.266	6.666	O	1.215	13.333	6.724	Ti	-9.684	14.855	3.347
Ti	-9.774	13.351	6.678	O	-9.751	14.824	5.231	O	-7.729	13.370	6.726
Ti	-3.159	14.828	3.354	Ti	-3.260	13.344	6.664	O	-3.265	14.838	5.241
O	-5.285	13.372	6.668	O	-1.229	13.332	6.669	O	1.221	10.388	6.728
Ti	-9.680	11.885	3.347	Ti	-9.751	10.388	6.692	O	-9.781	11.880	5.228
O	-7.752	10.427	6.613	Ti	-3.179	11.854	3.354	Ti	-3.226	10.381	6.728
O	-3.241	11.869	5.243	O	-5.277	10.440	6.667	O	-1.214	10.374	6.735
O	1.214	28.196	6.734	Ti	-9.806	28.172	6.726	O	-7.751	28.130	6.666
Ti	-3.282	28.175	6.692	O	-5.275	28.136	6.612	O	-1.221	28.183	6.730
O	1.229	25.236	6.668	Ti	-9.673	26.692	3.355	Ti	-9.775	25.208	6.664
O	-9.779	26.703	5.241	O	-7.744	25.196	6.669	Ti	-3.171	26.719	3.347
Ti	-3.261	25.214	6.677	O	-3.237	26.688	5.231	O	-5.299	25.197	6.724
O	-1.215	25.234	6.726	O	1.237	22.304	6.667	Ti	-9.693	23.719	3.354
Ti	-9.741	22.245	6.728	O	-9.755	23.734	5.243	O	-7.728	22.238	6.735

Ti	-3.166	23.749	3.347	Ti	-3.237	22.251	6.691	O	-3.268	23.744	5.227
O	-5.293	22.252	6.728	O	-1.239	22.291	6.612	O	-3.257	8.898	1.256
O	-9.771	8.898	1.256	O	-3.257	5.932	1.256	O	-9.771	5.932	1.256
Ti	0.000	8.898	0.000	Ti	-6.514	8.898	0.000	Ti	0.000	5.932	0.000
Ti	-6.514	5.932	0.000	O	-9.771	8.898	-7.787	O	-3.257	8.898	-7.787
O	-9.771	5.932	-7.787	O	-3.257	5.932	-7.787	Ti	-6.514	8.898	-6.514
Ti	0.000	8.898	-6.514	Ti	-6.514	5.932	-6.514	Ti	0.000	5.932	-6.514
Ti	-3.257	8.898	-3.257	Ti	-3.257	7.419	-0.009	O	-3.257	8.898	-1.274
O	-5.240	7.419	-0.009	O	-1.274	7.419	-0.009	O	1.274	7.419	-0.009
Ti	-9.771	8.898	-3.257	Ti	-9.771	7.419	-0.009	O	-9.771	8.898	-1.274
O	-7.787	7.419	-0.009	Ti	-3.257	5.932	-3.257	O	-3.257	5.932	-1.274
Ti	-9.771	5.932	-3.257	O	-9.771	5.932	-1.274	Ti	-6.514	7.419	-3.266
O	-6.514	8.898	-4.530	O	-6.514	8.898	-2.001	O	-8.497	7.419	-3.266
O	-4.530	7.419	-3.266	Ti	0.000	7.419	-3.266	O	0.000	8.898	-4.530
O	0.000	8.898	-2.001	O	-1.983	7.419	-3.266	O	1.983	7.419	-3.266
O	-6.514	5.932	-4.530	O	-6.514	5.932	-2.001	O	0.000	5.932	-4.530
O	0.000	5.932	-2.001	Ti	-9.771	7.419	-6.523	O	-9.771	8.898	-5.258
O	-7.787	7.419	-6.523	Ti	-3.257	7.419	-6.523	O	-3.257	8.898	-5.258
O	-5.240	7.419	-6.523	O	-1.274	7.419	-6.523	O	1.274	7.419	-6.523
O	-9.771	5.932	-5.258	O	-3.257	5.932	-5.258	O	-3.257	20.762	1.256
O	-9.771	20.762	1.256	O	-3.257	17.796	1.256	O	-9.771	17.796	1.256
O	-3.257	14.830	1.256	O	-9.771	14.830	1.256	O	-3.257	11.864	1.256
O	-9.771	11.864	1.256	O	-3.257	26.694	1.256	O	-9.771	26.694	1.256
O	-3.257	23.728	1.256	O	-9.771	23.728	1.256	Ti	0.000	20.762	0.000
Ti	-6.514	20.762	0.000	Ti	0.000	17.796	0.000	Ti	-6.514	17.796	0.000
Ti	0.000	14.830	0.000	Ti	-6.514	14.830	0.000	Ti	0.000	11.864	0.000
Ti	-6.514	11.864	0.000	Ti	0.000	26.694	0.000	Ti	-6.514	26.694	0.000
Ti	0.000	23.728	0.000	Ti	-6.514	23.728	0.000	O	-9.771	20.762	-7.787
O	-3.257	20.762	-7.787	O	-9.771	17.796	-7.787	O	-3.257	17.796	-7.787
O	-9.771	14.830	-7.787	O	-3.257	14.830	-7.787	O	-9.771	11.864	-7.787
O	-3.257	11.864	-7.787	O	-9.771	26.694	-7.787	O	-3.257	26.694	-7.787

O	-9.771	23.728	-7.787	O	-3.257	23.728	-7.787	Ti	-6.514	20.762	-6.514
Ti	-0.000	20.762	-6.514	Ti	-6.514	17.796	-6.514	Ti	-0.000	17.796	-6.514
Ti	-6.514	14.830	-6.514	Ti	-0.000	14.830	-6.514	Ti	-6.514	11.864	-6.514
Ti	-0.000	11.864	-6.514	Ti	-6.514	26.694	-6.514	Ti	0.000	26.694	-6.514
Ti	-6.514	23.728	-6.514	Ti	-0.000	23.728	-6.514	Ti	-3.257	20.762	-3.257
Ti	-3.257	19.283	-0.009	O	-3.257	20.762	-1.274	O	-5.240	19.283	-0.009
O	-1.274	19.283	-0.009	O	1.274	19.283	-0.009	Ti	-9.771	20.762	-3.257
Ti	-9.771	19.283	-0.009	O	-9.771	20.762	-1.274	O	-7.787	19.283	-0.009
Ti	-3.257	17.796	-3.257	Ti	-3.257	16.317	-0.009	O	-3.257	17.796	-1.274
O	-5.240	16.317	-0.009	O	-1.274	16.317	-0.009	O	1.274	16.317	-0.009
Ti	-9.771	17.796	-3.257	Ti	-9.771	16.317	-0.009	O	-9.771	17.796	-1.274
O	-7.787	16.317	-0.009	Ti	-3.257	14.830	-3.257	Ti	-3.257	13.351	-0.009
O	-3.257	14.830	-1.274	O	-5.240	13.351	-0.009	O	-1.274	13.351	-0.009
O	1.274	13.351	-0.009	Ti	-9.771	14.830	-3.257	Ti	-9.771	13.351	-0.009
O	-9.771	14.830	-1.274	O	-7.787	13.351	-0.009	Ti	-3.257	11.864	-3.257
Ti	-3.257	10.385	-0.009	O	-3.257	11.864	-1.274	O	-5.240	10.385	-0.009
O	-1.274	10.385	-0.009	O	1.274	10.385	-0.009	Ti	-9.771	11.864	-3.257
Ti	-9.771	10.385	-0.009	O	-9.771	11.864	-1.274	O	-7.787	10.385	-0.009
Ti	-3.257	28.181	-0.009	O	-5.240	28.181	-0.009	O	-1.274	28.181	-0.009
O	1.274	28.181	-0.009	Ti	-9.771	28.181	-0.009	O	-7.787	28.181	-0.009
Ti	-3.257	26.694	-3.257	Ti	-3.257	25.215	-0.009	O	-3.257	26.694	-1.274
O	-5.240	25.215	-0.009	O	-1.274	25.215	-0.009	O	1.274	25.215	-0.009
Ti	-9.771	26.694	-3.257	Ti	-9.771	25.215	-0.009	O	-9.771	26.694	-1.274
O	-7.787	25.215	-0.009	Ti	-3.257	23.728	-3.257	Ti	-3.257	22.249	-0.009
O	-3.257	23.728	-1.274	O	-5.240	22.249	-0.009	O	-1.274	22.249	-0.009
O	1.274	22.249	-0.009	Ti	-9.771	23.728	-3.257	Ti	-9.771	22.249	-0.009
O	-9.771	23.728	-1.274	O	-7.787	22.249	-0.009	Ti	-6.514	19.283	-3.266
O	-6.514	20.762	-4.530	O	-6.514	20.762	-2.001	O	-8.497	19.283	-3.266
O	-4.530	19.283	-3.266	Ti	-0.000	19.283	-3.266	O	-0.000	20.762	-4.530
O	-0.000	20.762	-2.001	O	-1.983	19.283	-3.266	O	1.983	19.283	-3.266
Ti	-6.514	16.317	-3.266	O	-6.514	17.796	-4.530	O	-6.514	17.796	-2.001

O	-8.497	16.317	-3.266	O	-4.530	16.317	-3.266	Ti	-0.000	16.317	-3.266
O	-0.000	17.796	-4.530	O	-0.000	17.796	-2.001	O	-1.983	16.317	-3.266
O	1.983	16.317	-3.266	Ti	-6.514	13.351	-3.266	O	-6.514	14.830	-4.530
O	-6.514	14.830	-2.001	O	-8.497	13.351	-3.266	O	-4.530	13.351	-3.266
Ti	-0.000	13.351	-3.266	O	-0.000	14.830	-4.530	O	-0.000	14.830	-2.001
O	-1.983	13.351	-3.266	O	1.983	13.351	-3.266	Ti	-6.514	10.385	-3.266
O	-6.514	11.864	-4.530	O	-6.514	11.864	-2.001	O	-8.497	10.385	-3.266
O	-4.530	10.385	-3.266	Ti	-0.000	10.385	-3.266	O	-0.000	11.864	-4.530
O	-0.000	11.864	-2.001	O	-1.983	10.385	-3.266	O	1.983	10.385	-3.266
Ti	-6.514	28.181	-3.266	O	-8.497	28.181	-3.266	O	-4.530	28.181	-3.266
Ti	0.000	28.181	-3.266	O	-1.983	28.181	-3.266	O	1.983	28.181	-3.266
Ti	-6.514	25.215	-3.266	O	-6.514	26.694	-4.530	O	-6.514	26.694	-2.001
O	-8.497	25.215	-3.266	O	-4.530	25.215	-3.266	Ti	0.000	25.215	-3.266
O	0.000	26.694	-4.530	O	0.000	26.694	-2.001	O	-1.983	25.215	-3.266
O	1.983	25.215	-3.266	Ti	-6.514	22.249	-3.266	O	-6.514	23.728	-4.530
O	-6.514	23.728	-2.001	O	-8.497	22.249	-3.266	O	-4.530	22.249	-3.266
Ti	-0.000	22.249	-3.266	O	-0.000	23.728	-4.530	O	-0.000	23.728	-2.001
O	-1.983	22.249	-3.266	O	1.983	22.249	-3.266	Ti	-9.771	19.283	-6.523
O	-9.771	20.762	-5.258	O	-7.787	19.283	-6.523	Ti	-3.257	19.283	-6.523
O	-3.257	20.762	-5.258	O	-5.240	19.283	-6.523	O	-1.274	19.283	-6.523
O	1.274	19.283	-6.523	Ti	-9.771	16.317	-6.523	O	-9.771	17.796	-5.258
O	-7.787	16.317	-6.523	Ti	-3.257	16.317	-6.523	O	-3.257	17.796	-5.258
O	-5.240	16.317	-6.523	O	-1.274	16.317	-6.523	O	1.274	16.317	-6.523
Ti	-9.771	13.351	-6.523	O	-9.771	14.830	-5.258	O	-7.787	13.351	-6.523
Ti	-3.257	13.351	-6.523	O	-3.257	14.830	-5.258	O	-5.240	13.351	-6.523
O	-1.274	13.351	-6.523	O	1.274	13.351	-6.523	Ti	-9.771	10.385	-6.523
O	-9.771	11.864	-5.258	O	-7.787	10.385	-6.523	Ti	-3.257	10.385	-6.523
O	-3.257	11.864	-5.258	O	-5.240	10.385	-6.523	O	-1.274	10.385	-6.523
O	1.274	10.385	-6.523	Ti	-9.771	28.181	-6.523	O	-7.787	28.181	-6.523
Ti	-3.257	28.181	-6.523	O	-5.240	28.181	-6.523	O	-1.274	28.181	-6.523
O	1.274	28.181	-6.523	Ti	-9.771	25.215	-6.523	O	-9.771	26.694	-5.258

O	-7.787	25.215	-6.523	Ti	-3.257	25.215	-6.523	O	-3.257	26.694	-5.258
O	-5.240	25.215	-6.523	O	-1.274	25.215	-6.523	O	1.274	25.215	-6.523
Ti	-9.771	22.249	-6.523	O	-9.771	23.728	-5.258	O	-7.787	22.249	-6.523
Ti	-3.257	22.249	-6.523	O	-3.257	23.728	-5.258	O	-5.240	22.249	-6.523
O	-1.274	22.249	-6.523	O	1.274	22.249	-6.523				

Table S4: Pyr monolayer on rutile TiO_2 (110) surface

C	-10.462	16.267	10.517	C	-10.038	17.608	10.676	C	-8.696	17.871	10.893
C	-7.784	16.813	10.877	C	-8.271	15.511	10.696	C	-9.531	9.085	10.670
C	-9.108	10.426	10.513	C	-7.725	10.713	10.144	C	-7.041	9.725	9.451
C	-7.096	11.998	10.153	C	-7.340	14.390	10.464	C	-6.005	14.581	10.138
C	-5.210	13.468	9.824	C	-5.732	12.193	9.828	H	-8.354	18.895	11.027
H	-6.721	17.000	10.996	H	-8.808	8.276	10.588	H	-8.853	12.923	10.576
H	-5.586	15.579	10.060	H	-4.185	13.640	9.514	H	-5.113	11.344	9.545
N	-9.589	15.233	10.604	N	-9.980	11.461	10.602	N	-7.834	13.115	10.461
N	-6.470	8.964	8.750	C	-0.813	14.503	9.843	C	-1.336	13.228	9.843
C	-0.540	12.115	10.151	C	0.797	12.304	10.468	C	0.553	14.697	10.159
C	1.183	15.981	10.148	C	0.503	16.970	9.453	C	1.730	11.183	10.695
C	1.243	9.880	10.875	C	2.155	8.822	10.888	H	-1.433	15.354	9.564
H	-2.364	13.058	9.541	H	-0.961	11.117	10.077	H	2.312	13.770	10.573
H	2.266	18.417	10.596	H	0.180	9.693	10.996	H	1.812	7.798	11.021
N	1.292	13.579	10.462	N	-0.058	17.736	8.749	C	-7.309	26.369	9.834
C	-7.831	25.093	9.831	C	-7.035	23.981	10.143	C	-5.700	24.171	10.466
C	-5.944	26.563	10.156	C	-5.315	27.848	10.145	C	-5.997	28.836	9.452
C	-3.931	28.134	10.513	C	-1.253	28.681	10.869	C	-1.740	27.378	10.692
C	-4.768	23.050	10.697	C	-5.255	21.748	10.880	C	-4.343	20.690	10.893
C	-3.001	20.953	10.675	C	-2.578	22.294	10.516	C	-1.195	22.579	10.146
C	-0.513	21.591	9.452	C	-0.564	23.864	10.157	C	-0.808	26.257	10.464
C	0.528	26.446	10.145	C	1.325	25.332	9.838	C	0.802	24.057	9.840
H	-7.928	27.218	9.552	H	-8.857	24.922	9.523	H	-7.455	22.982	10.065
H	-4.187	25.638	10.578	H	-6.318	21.561	11.002	H	-4.685	19.666	11.029
H	-2.278	20.144	10.595	H	-2.322	24.791	10.571	H	0.949	27.443	10.069
H	2.352	25.503	9.535	H	1.422	23.207	9.562	N	-5.206	25.446	10.464
N	-3.058	27.100	10.602	N	-3.450	23.328	10.602	N	-1.302	24.982	10.461
N	0.052	20.827	8.750	C	-3.507	5.747	10.668	C	-2.165	6.011	10.883
H	-4.230	6.557	10.586	H	-1.822	7.035	11.014	H	-0.189	5.140	10.987

N	-6.563	5.871	8.749	O	-9.749	8.907	7.795	O	-3.279	8.903	7.818
O	-9.754	5.933	7.815	O	-3.285	5.928	7.798	Ti	-6.408	8.898	6.558
Ti	0.050	8.909	6.366	Ti	-6.624	5.944	6.557	Ti	-0.055	5.933	6.366
Ti	0.092	7.419	3.173	O	-0.000	8.905	2.003	O	0.008	8.903	4.561
O	-1.957	7.432	3.268	O	1.958	7.416	3.262	Ti	-6.421	7.420	3.345
O	-6.512	8.881	2.019	O	-6.493	8.923	4.590	O	-8.485	7.427	3.288
O	-4.540	7.421	3.290	O	-0.003	5.935	2.003	O	-0.007	5.937	4.561
O	-6.509	5.963	2.019	O	-6.524	5.921	4.590	O	1.215	7.410	6.737
Ti	-9.699	8.904	3.370	Ti	-9.791	7.420	6.723	O	-9.819	8.903	5.240
O	-7.756	7.450	6.608	Ti	-3.188	8.905	3.378	Ti	-3.244	7.410	6.724
O	-3.238	8.912	5.256	O	-5.274	7.388	6.610	O	-1.217	7.433	6.738
Ti	-9.695	5.939	3.379	O	-9.783	5.930	5.253	Ti	-3.178	5.945	3.368
O	-3.202	5.938	5.247	O	-9.793	20.767	7.818	O	-3.235	20.771	7.796
O	-9.797	17.793	7.799	O	-3.239	17.797	7.815	O	-9.779	14.831	7.795
O	-3.256	14.821	7.801	O	-9.764	11.868	7.793	O	-3.262	11.879	7.802
O	-9.769	26.685	7.802	O	-3.265	26.695	7.795	O	-9.775	23.743	7.802
O	-3.250	23.732	7.793	Ti	-6.463	20.773	6.366	Ti	0.108	20.762	6.558
Ti	-6.569	17.797	6.366	Ti	-0.112	17.808	6.557	Ti	-6.501	14.829	6.355
Ti	0.033	14.833	6.326	Ti	-6.553	11.871	6.327	Ti	-0.019	11.876	6.354
Ti	-6.482	26.697	6.326	Ti	0.013	26.694	6.355	Ti	-6.533	23.740	6.354
Ti	-0.040	23.735	6.327	Ti	0.093	19.284	3.346	O	0.003	20.745	2.019
O	0.021	20.787	4.591	O	-1.971	19.291	3.288	O	1.974	19.285	3.290
Ti	-6.422	19.283	3.173	O	-6.514	20.769	2.003	O	-6.506	20.767	4.561
O	-8.471	19.295	3.268	O	-4.556	19.281	3.262	Ti	0.099	16.393	3.205
O	0.005	17.828	2.019	O	-0.010	17.785	4.590	O	-1.966	16.320	3.270
O	1.973	16.325	3.272	Ti	-6.404	16.302	3.188	O	-6.517	17.799	2.003
O	-6.521	17.801	4.561	O	-8.473	16.321	3.263	O	-4.553	16.324	3.263
Ti	0.109	13.390	3.149	O	0.001	14.855	1.994	O	0.003	14.822	4.530
O	-1.961	13.355	3.263	O	1.965	13.357	3.255	Ti	-6.403	13.314	3.151
O	-6.513	14.836	1.996	O	-6.517	14.837	4.549	O	-8.475	13.357	3.261
O	-4.548	13.357	3.258	Ti	0.107	10.402	3.188	O	-0.002	11.869	1.996

O	0.003	11.868	4.548	O	-1.960	10.389	3.268	O	1.960	10.395	3.257
Ti	-6.428	10.312	3.205	O	-6.512	11.853	1.994	O	-6.520	11.885	4.531
O	-8.480	10.388	3.273	O	-4.543	10.397	3.268	Ti	0.110	28.166	3.188
O	-1.959	28.185	3.263	O	1.961	28.188	3.263	Ti	-6.414	28.257	3.205
O	-8.480	28.184	3.270	O	-4.541	28.189	3.272	Ti	0.111	25.178	3.151
O	0.000	26.700	1.996	O	-0.003	26.701	4.549	O	-1.961	25.221	3.261
O	1.966	25.221	3.258	Ti	-6.404	25.254	3.149	O	-6.513	26.719	1.994
O	-6.512	26.686	4.530	O	-8.475	25.219	3.263	O	-4.549	25.221	3.255
Ti	0.085	22.176	3.205	O	0.001	23.717	1.994	O	-0.007	23.749	4.531
O	-1.966	22.251	3.273	O	1.971	22.262	3.268	Ti	-6.407	22.266	3.188
O	-6.516	23.732	1.996	O	-6.511	23.732	4.548	O	-8.474	22.252	3.268
O	-4.553	22.259	3.257	O	1.240	19.251	6.610	Ti	-9.702	20.769	3.378
Ti	-9.757	19.274	6.724	O	-9.751	20.776	5.256	O	-7.731	19.297	6.738
Ti	-3.186	20.768	3.371	Ti	-3.277	19.284	6.724	O	-3.305	20.767	5.241
O	-5.298	19.274	6.737	O	-1.242	19.315	6.609	O	1.233	16.276	6.626
Ti	-9.692	17.809	3.368	Ti	-9.801	16.308	6.696	O	-9.716	17.801	5.247
O	-7.736	16.320	6.730	Ti	-3.181	17.804	3.379	Ti	-3.295	16.311	6.723
O	-3.269	17.794	5.253	O	-5.302	16.330	6.735	O	-1.240	16.264	6.662
O	1.214	13.333	6.731	Ti	-9.685	14.851	3.357	Ti	-9.775	13.351	6.711
O	-9.756	14.825	5.239	O	-7.729	13.370	6.732	Ti	-3.160	14.828	3.351
Ti	-3.260	13.345	6.654	O	-3.266	14.836	5.238	O	-5.286	13.372	6.668
O	-1.229	13.332	6.669	O	1.221	10.387	6.728	Ti	-9.683	11.883	3.358
Ti	-9.749	10.391	6.694	O	-9.779	11.878	5.235	O	-7.749	10.423	6.620
Ti	-3.180	11.854	3.350	Ti	-3.225	10.380	6.726	O	-3.240	11.871	5.240
O	-5.276	10.442	6.665	O	-1.214	10.375	6.737	O	1.212	28.194	6.736
Ti	-9.809	28.176	6.724	O	-7.753	28.128	6.663	Ti	-3.287	28.172	6.695
O	-5.281	28.140	6.622	O	-1.222	28.184	6.730	O	1.227	25.236	6.669
Ti	-9.673	26.692	3.351	Ti	-9.775	25.210	6.654	O	-9.781	26.701	5.238
O	-7.743	25.196	6.669	Ti	-3.171	26.715	3.357	Ti	-3.261	25.215	6.711
O	-3.242	26.689	5.239	O	-5.300	25.198	6.731	O	-1.216	25.234	6.733
O	1.238	22.307	6.664	Ti	-9.694	23.718	3.351	Ti	-9.739	22.244	6.726

O	-9.754	23.735	5.240	O	-7.728	22.239	6.737	Ti	-3.169	23.747	3.358
Ti	-3.235	22.254	6.695	O	-3.264	23.742	5.236	O	-5.293	22.251	6.728
O	-1.234	22.287	6.623	O	-3.257	8.898	1.256	O	-9.771	8.898	1.256
O	-3.257	5.932	1.256	O	-9.771	5.932	1.256	Ti	0.000	8.898	0.000
Ti	-6.514	8.898	0.000	Ti	0.000	5.932	0.000	Ti	-6.514	5.932	0.000
O	-9.771	8.898	-7.787	O	-3.257	8.898	-7.787	O	-9.771	5.932	-7.787
O	-3.257	5.932	-7.787	Ti	-6.514	8.898	-6.514	Ti	0.000	8.898	-6.514
Ti	-6.514	5.932	-6.514	Ti	0.000	5.932	-6.514	Ti	-3.257	8.898	-3.257
Ti	-3.257	7.419	-0.009	O	-3.257	8.898	-1.274	O	-5.240	7.419	-0.009
O	-1.274	7.419	-0.009	O	1.274	7.419	-0.009	Ti	-9.771	8.898	-3.257
Ti	-9.771	7.419	-0.009	O	-9.771	8.898	-1.274	O	-7.787	7.419	-0.009
Ti	-3.257	5.932	-3.257	O	-3.257	5.932	-1.274	Ti	-9.771	5.932	-3.257
O	-9.771	5.932	-1.274	Ti	-6.514	7.419	-3.266	O	-6.514	8.898	-4.530
O	-6.514	8.898	-2.001	O	-8.497	7.419	-3.266	O	-4.530	7.419	-3.266
Ti	0.000	7.419	-3.266	O	0.000	8.898	-4.530	O	0.000	8.898	-2.001
O	-1.983	7.419	-3.266	O	1.983	7.419	-3.266	O	-6.514	5.932	-4.530
O	-6.514	5.932	-2.001	O	0.000	5.932	-4.530	O	0.000	5.932	-2.001
Ti	-9.771	7.419	-6.523	O	-9.771	8.898	-5.258	O	-7.787	7.419	-6.523
Ti	-3.257	7.419	-6.523	O	-3.257	8.898	-5.258	O	-5.240	7.419	-6.523
O	-1.274	7.419	-6.523	O	1.274	7.419	-6.523	O	-9.771	5.932	-5.258
O	-3.257	5.932	-5.258	O	-3.257	20.762	1.256	O	-9.771	20.762	1.256
O	-3.257	17.796	1.256	O	-9.771	17.796	1.256	O	-3.257	14.830	1.256
O	-9.771	14.830	1.256	O	-3.257	11.864	1.256	O	-9.771	11.864	1.256
O	-3.257	26.694	1.256	O	-9.771	26.694	1.256	O	-3.257	23.728	1.256
O	-9.771	23.728	1.256	Ti	0.000	20.762	0.000	Ti	-6.514	20.762	0.000
Ti	0.000	17.796	0.000	Ti	-6.514	17.796	0.000	Ti	0.000	14.830	0.000
Ti	-6.514	14.830	0.000	Ti	0.000	11.864	0.000	Ti	-6.514	11.864	0.000
Ti	0.000	26.694	0.000	Ti	-6.514	26.694	0.000	Ti	0.000	23.728	0.000
Ti	-6.514	23.728	0.000	O	-9.771	20.762	-7.787	O	-3.257	20.762	-7.787
O	-9.771	17.796	-7.787	O	-3.257	17.796	-7.787	O	-9.771	14.830	-7.787
O	-3.257	14.830	-7.787	O	-9.771	11.864	-7.787	O	-3.257	11.864	-7.787

O	-9.771	26.694	-7.787	O	-3.257	26.694	-7.787	O	-9.771	23.728	-7.787
O	-3.257	23.728	-7.787	Ti	-6.514	20.762	-6.514	Ti	-0.000	20.762	-6.514
Ti	-6.514	17.796	-6.514	Ti	-0.000	17.796	-6.514	Ti	-6.514	14.830	-6.514
Ti	-0.000	14.830	-6.514	Ti	-6.514	11.864	-6.514	Ti	-0.000	11.864	-6.514
Ti	-6.514	26.694	-6.514	Ti	0.000	26.694	-6.514	Ti	-6.514	23.728	-6.514
Ti	-0.000	23.728	-6.514	Ti	-3.257	20.762	-3.257	Ti	-3.257	19.283	-0.009
O	-3.257	20.762	-1.274	O	-5.240	19.283	-0.009	O	-1.274	19.283	-0.009
O	1.274	19.283	-0.009	Ti	-9.771	20.762	-3.257	Ti	-9.771	19.283	-0.009
O	-9.771	20.762	-1.274	O	-7.787	19.283	-0.009	Ti	-3.257	17.796	-3.257
Ti	-3.257	16.317	-0.009	O	-3.257	17.796	-1.274	O	-5.240	16.317	-0.009
O	-1.274	16.317	-0.009	O	1.274	16.317	-0.009	Ti	-9.771	17.796	-3.257
Ti	-9.771	16.317	-0.009	O	-9.771	17.796	-1.274	O	-7.787	16.317	-0.009
Ti	-3.257	14.830	-3.257	Ti	-3.257	13.351	-0.009	O	-3.257	14.830	-1.274
O	-5.240	13.351	-0.009	O	-1.274	13.351	-0.009	O	1.274	13.351	-0.009
Ti	-9.771	14.830	-3.257	Ti	-9.771	13.351	-0.009	O	-9.771	14.830	-1.274
O	-7.787	13.351	-0.009	Ti	-3.257	11.864	-3.257	Ti	-3.257	10.385	-0.009
O	-3.257	11.864	-1.274	O	-5.240	10.385	-0.009	O	-1.274	10.385	-0.009
O	1.274	10.385	-0.009	Ti	-9.771	11.864	-3.257	Ti	-9.771	10.385	-0.009
O	-9.771	11.864	-1.274	O	-7.787	10.385	-0.009	Ti	-3.257	28.181	-0.009
O	-5.240	28.181	-0.009	O	-1.274	28.181	-0.009	O	1.274	28.181	-0.009
Ti	-9.771	28.181	-0.009	O	-7.787	28.181	-0.009	Ti	-3.257	26.694	-3.257
Ti	-3.257	25.215	-0.009	O	-3.257	26.694	-1.274	O	-5.240	25.215	-0.009
O	-1.274	25.215	-0.009	O	1.274	25.215	-0.009	Ti	-9.771	26.694	-3.257
Ti	-9.771	25.215	-0.009	O	-9.771	26.694	-1.274	O	-7.787	25.215	-0.009
Ti	-3.257	23.728	-3.257	Ti	-3.257	22.249	-0.009	O	-3.257	23.728	-1.274
O	-5.240	22.249	-0.009	O	-1.274	22.249	-0.009	O	1.274	22.249	-0.009
Ti	-9.771	23.728	-3.257	Ti	-9.771	22.249	-0.009	O	-9.771	23.728	-1.274
O	-7.787	22.249	-0.009	Ti	-6.514	19.283	-3.266	O	-6.514	20.762	-4.530
O	-6.514	20.762	-2.001	O	-8.497	19.283	-3.266	O	-4.530	19.283	-3.266
Ti	-0.000	19.283	-3.266	O	-0.000	20.762	-4.530	O	-0.000	20.762	-2.001
O	-1.983	19.283	-3.266	O	1.983	19.283	-3.266	Ti	-6.514	16.317	-3.266

O	-6.514	17.796	-4.530	O	-6.514	17.796	-2.001	O	-8.497	16.317	-3.266
O	-4.530	16.317	-3.266	Ti	-0.000	16.317	-3.266	O	-0.000	17.796	-4.530
O	-0.000	17.796	-2.001	O	-1.983	16.317	-3.266	O	1.983	16.317	-3.266
Ti	-6.514	13.351	-3.266	O	-6.514	14.830	-4.530	O	-6.514	14.830	-2.001
O	-8.497	13.351	-3.266	O	-4.530	13.351	-3.266	Ti	-0.000	13.351	-3.266
O	-0.000	14.830	-4.530	O	-0.000	14.830	-2.001	O	-1.983	13.351	-3.266
O	1.983	13.351	-3.266	Ti	-6.514	10.385	-3.266	O	-6.514	11.864	-4.530
O	-6.514	11.864	-2.001	O	-8.497	10.385	-3.266	O	-4.530	10.385	-3.266
Ti	-0.000	10.385	-3.266	O	-0.000	11.864	-4.530	O	-0.000	11.864	-2.001
O	-1.983	10.385	-3.266	O	1.983	10.385	-3.266	Ti	-6.514	28.181	-3.266
O	-8.497	28.181	-3.266	O	-4.530	28.181	-3.266	Ti	0.000	28.181	-3.266
O	-1.983	28.181	-3.266	O	1.983	28.181	-3.266	Ti	-6.514	25.215	-3.266
O	-6.514	26.694	-4.530	O	-6.514	26.694	-2.001	O	-8.497	25.215	-3.266
O	-4.530	25.215	-3.266	Ti	0.000	25.215	-3.266	O	0.000	26.694	-4.530
O	0.000	26.694	-2.001	O	-1.983	25.215	-3.266	O	1.983	25.215	-3.266
Ti	-6.514	22.249	-3.266	O	-6.514	23.728	-4.530	O	-6.514	23.728	-2.001
O	-8.497	22.249	-3.266	O	-4.530	22.249	-3.266	Ti	-0.000	22.249	-3.266
O	-0.000	23.728	-4.530	O	-0.000	23.728	-2.001	O	-1.983	22.249	-3.266
O	1.983	22.249	-3.266	Ti	-9.771	19.283	-6.523	O	-9.771	20.762	-5.258
O	-7.787	19.283	-6.523	Ti	-3.257	19.283	-6.523	O	-3.257	20.762	-5.258
O	-5.240	19.283	-6.523	O	-1.274	19.283	-6.523	O	1.274	19.283	-6.523
Ti	-9.771	16.317	-6.523	O	-9.771	17.796	-5.258	O	-7.787	16.317	-6.523
Ti	-3.257	16.317	-6.523	O	-3.257	17.796	-5.258	O	-5.240	16.317	-6.523
O	-1.274	16.317	-6.523	O	1.274	16.317	-6.523	Ti	-9.771	13.351	-6.523
O	-9.771	14.830	-5.258	O	-7.787	13.351	-6.523	Ti	-3.257	13.351	-6.523
O	-3.257	14.830	-5.258	O	-5.240	13.351	-6.523	O	-1.274	13.351	-6.523
O	1.274	13.351	-6.523	Ti	-9.771	10.385	-6.523	O	-9.771	11.864	-5.258
O	-7.787	10.385	-6.523	Ti	-3.257	10.385	-6.523	O	-3.257	11.864	-5.258
O	-5.240	10.385	-6.523	O	-1.274	10.385	-6.523	O	1.274	10.385	-6.523
Ti	-9.771	28.181	-6.523	O	-7.787	28.181	-6.523	Ti	-3.257	28.181	-6.523
O	-5.240	28.181	-6.523	O	-1.274	28.181	-6.523	O	1.274	28.181	-6.523

Ti	-9.771	25.215	-6.523	O	-9.771	26.694	-5.258	O	-7.787	25.215	-6.523
Ti	-3.257	25.215	-6.523	O	-3.257	26.694	-5.258	O	-5.240	25.215	-6.523
O	-1.274	25.215	-6.523	O	1.274	25.215	-6.523	Ti	-9.771	22.249	-6.523
O	-9.771	23.728	-5.258	O	-7.787	22.249	-6.523	Ti	-3.257	22.249	-6.523
O	-3.257	23.728	-5.258	O	-5.240	22.249	-6.523	O	-1.274	22.249	-6.523
O	1.274	22.249	-6.523								

References

[1] Y. Gurdal, S. Luber, J. Hutter, and M. Iannuzzi, Phys. Chem. Chem. Phys. **17**, 22846 (2015).

[2] J. Tersoff and D. R. Hamann, Phys. Rev. B **31**, 805 (1985).

[3] G. Lovat, D. Forrer, M. Abadia, M. Dominguez, M. Casarin, C. Rogero, A. Vittadini, and L. Floreano, Phys. Chem. Chem. Phys. **17**, 30119 (2015).

[4] R. F. W. Bader and C. F. Matta, J. Phys. Chem. A **108**, 8385 (2004).