Supplementary Material (ESI) for *PCCP*

Supporting information for:

The role of van der Waals interactions in surface-supported supramolecular networks

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1. Single molecules on Au(111)

In this section we describe DFT calculations used to determine the preferred adsorption sites for single DATP and PTCDA on Au(111).

To determine the most stable adsorption configurations for the DATP and PTCDEA molecules we performed geometry optimization starting from "adequate" guess configurations. For molecules containing functional groups, the stable positions are usually associated with the positions of these groups with respect to the surface. In the case of fcc(111) surfaces, four high-symmetry positions are usually referred to for describing adsorption geometries. Additionally, due to the high symmetry of Au(111), we can choose some special points as references, namely, *top*, *bridge*, *hcp*-hollow, *fcc*-hollow that correspond to positions directly *on top* of a surface atom, the *middle* between two surface atoms, on top of a second layer atom and on top of a third layer atom, respectively. These high-symmetry adsorption sites are schematically shown in figure S1.

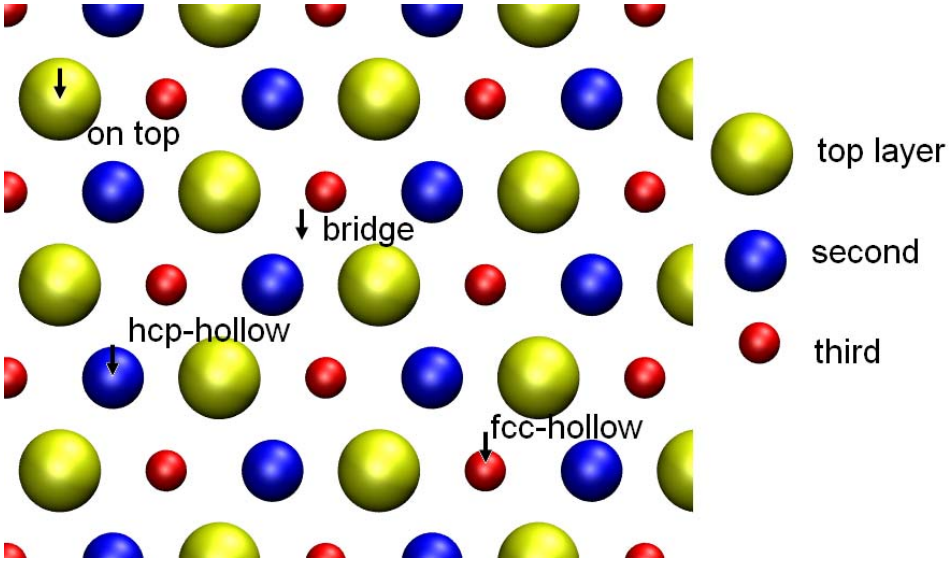

Figure S1. Reference high symmetry adsorption sites for the Au(111) surface.

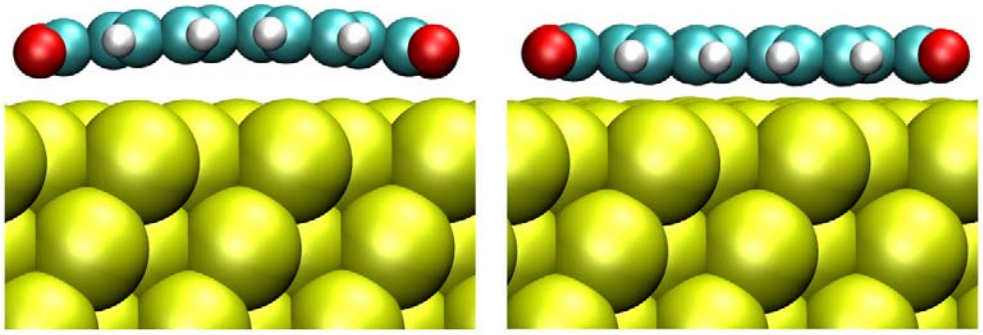

Figure S2. Geometry of PTCDA on Au(111) obtained with PBE (left) and PBE-D (right) simulations.

Our models are obtained by placing PTCDA on Au(111) such that carboxylic oxygen atoms are located at the top (bridge, hcp, fcc) positions. In the same fashion, DATP is located referring to the position of its N atoms. We optimize these models on Au(111) with PBE and PBE-D. The resulting binding energies are presented in table S1.

		on-top	bridge	hcp	Fcc
DATP / Au(111)	ΔE_{DFT} (eV)	-0.37	-0.29	-0.22	-0.22
	ΔE_{PBE-D} (eV)	-2.06	-2.0	-1.96	-1.95
PTCDA / Au(111)	ΔE_{DFT} (eV)	-0.04	-0.03	0.0	-0.01
	ΔE_{PBE-D} (eV)	-1.92	-1.89	-1.87	-1.87

Table S1. Adsorption site dependence of the binding energy of PTCDA and DATP on Au(111).

We find that for PTCDA and DATP, the on-top position is the most favorable one. PBE and PBE–D geometries of PTCDA on Au are shown in figure S2. The bridge–like geometry of PTCDA in the PBE simulation is not compatible with the experimental suggestion [S1,S2], whereas the PBE–D result is in agreement. In Figure S3a and S3b we plot the projected density of states (PDOS) for the PTCDA and DATP molecules on Au(111) (projection on a subset of atomic orbitals centered on the positions of the atoms of the molecules).

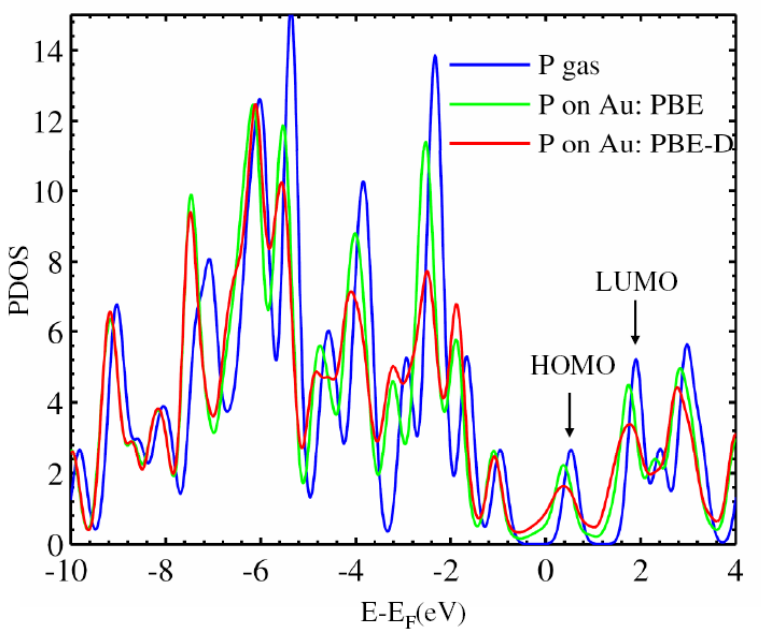

Figure S3a. Projected DOS on the molecular atoms for isolated PTCDA (P) in vacuum (in this case it is the total DOS) and on Au(111).

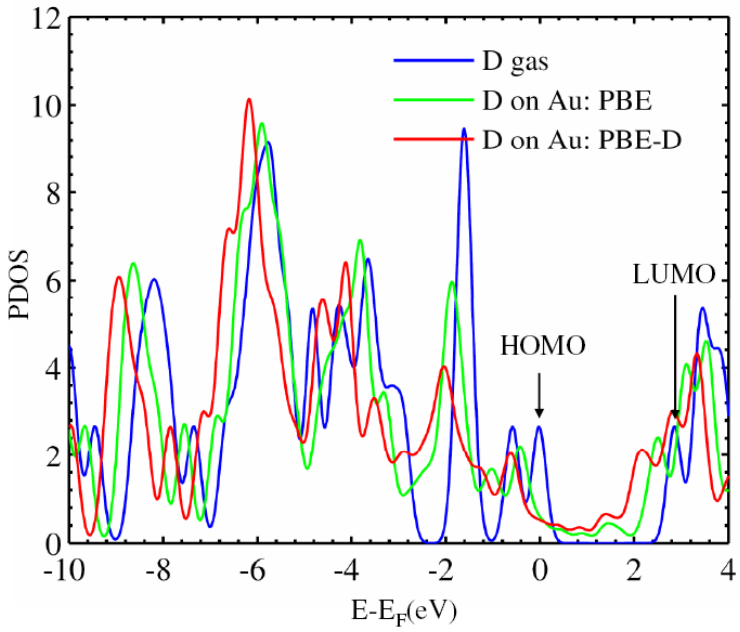

Figure S3b. Projected DOS on the molecular atoms of isolated DATP (D) in vacuum and on Au(111).

Comparison of gas phase, PBE and PBE-D results shows that molecular characteristics of PTCDA are only slightly modified due to Pauli repulsion. In the case of DATP a strong

modification is found, with the sharpest peak at E = –1.16 eV being strongly reduced. This change is mainly due to nitrogen states (not shown).

2. Homomolecular assemblies

Homomolecular nanostructures for PTCDA and for DATP on Au(111) have been reported in [S3]. The corresponding STM images and structures are shown in figure S4.

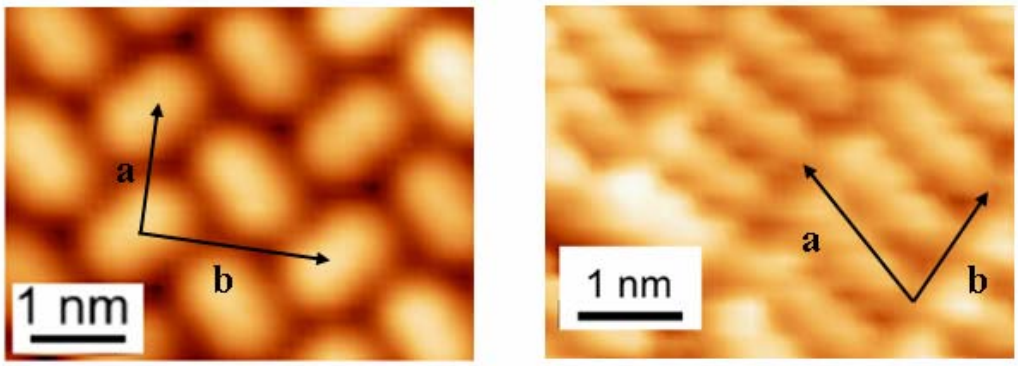

Figure S4. STM images of homomolecular networks of PTCDA and DATP on Au(111).

For the simulations of the networks we adopted unit cells containing two molecules. For PTCDA we used a rectangular 12.6×19.5Å^2 unit cell, very close to the experimental one (12.4×19.7 Å^2) [2]. The initial angle between two molecules in a unit cell, about 85°, is almost unchanged after completion of the geometry optimization. Also in the case of DATP networks our simulation cell defined by two vectors **a** and **b** and the angle θ between them, with a=15.7 Å , b=13.2 Å and θ = 78.5° is also close to the experimental one, a=15.8 Å, b=13.0 Å, θ = 78.5° .

3. Electronic properties of the bimolecular superstructure

In the supramolecular assemblies on Au(111), each PTCDA experiences the interaction with the surface and its four nearest neighbors (and, to a lesser extent, with next nearest neighbors due to long range interactions). Its electronic structure is therefore strongly modified with respect to the isolated molecule.

The coordinates of the optimized structure (at the PBE-D level) are given in Table S3.

In figures S5 and S6 we show the PDOS on PTCDA and DATP in the bimolecular network in vacuum and on Au(111).

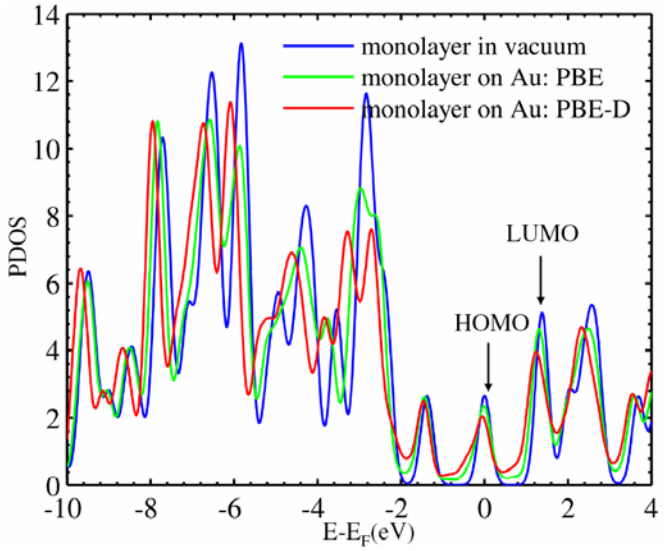

Figure S5. Projected DOS of PTCDA in PTCDA–DATP network in vacuum (with geometry taken from the relaxed PTCDA–DATP/Au system) and on Au(111).

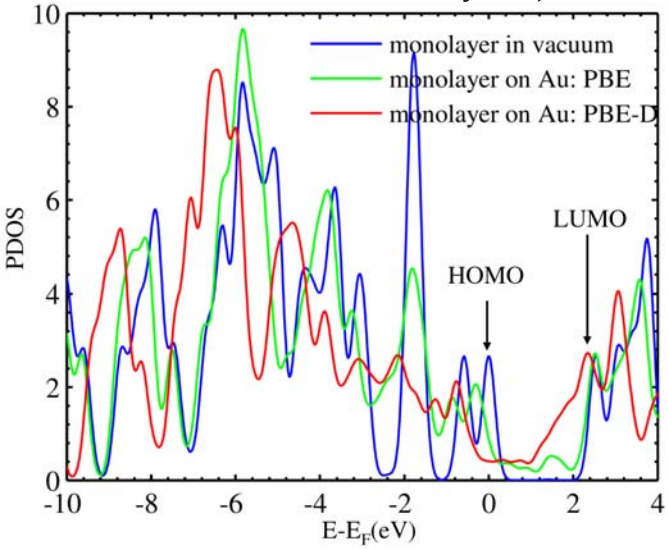

Figure S6. Projected DOS of DATP in PTCDA–DATP network in vacuum (with geometry taken from the relaxed PTCDA–DATP/Au system) and on Au(111).

The effect of hydrogen bonding on the electronic structure of PTCDA is evident. For example, the sharp peak at about −1.6 eV (figure S3a) nearly disappears (figure S5). This can be understood from the fact that the corresponding states are mostly concentrated on the oxygens. In terms of hydrogen bonding, all carboxylic oxygen atoms gain charge, and this strongly modifies the electronic states and the spatial electronic distribution of the network with respect to the isolated molecule (Figure S7). The electronic structure of DATP is instead somewhat modified by the N–H···O hydrogen bonds (the C–H···O bonds are less important, see figure S7). Four H atoms in these bonds lose charge, and there is a redistribution of electrons around the ends of the molecules. However, since the states around -2 eV are strongly delocalized over the molecule, the

modifications in this energy region due to hydrogen bonding are less evident than in the case of PTCDA.

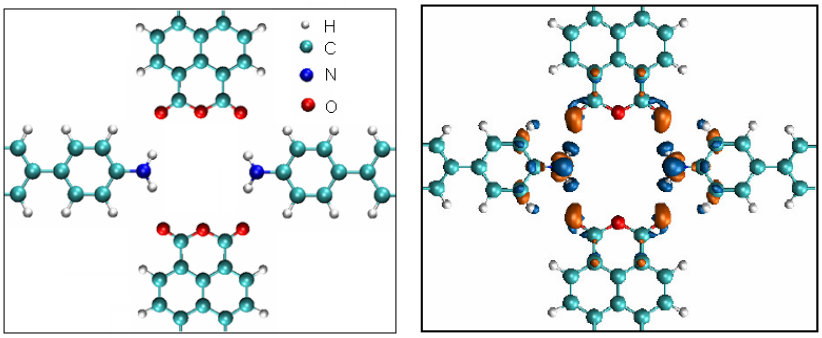

Figure S7. Left panel. Atomic sites: two hydrogen bonds in each PTCDA-DATP junction, namely C–O···H(–N) and C–O···H(–C). Right panel. Charge difference *iso*-surface of the monolayer *in vacuum* at 0.007 e/Å^3 with accumulation (orange) and depletion (blue).

Figure S8 shows the electron distribution map in a plane crossing carboxylic oxygen atoms of the monolayer on the substrate.

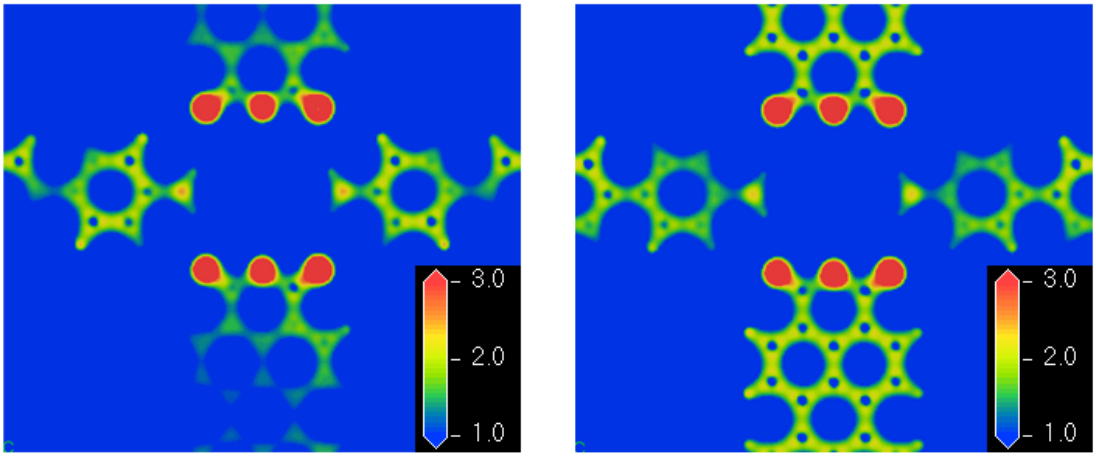

Figure S8. Electron distribution map within the plane crossing carboxylic oxygen atoms in the monolayer on Au(111) in DFT(left) and PBE-D(right) simulations. The role of van der Waals interactions in making the system planar is evident from the comparison of both diagrams. Indeed, on the right panel (PBE-D), the rotation of the central DATP ring (left panel, PBE) is not present anymore; moreover, PTCDA is fully planar within PBE-D (as experimentally observed) which is reflected in the arrangement of the bonding charge.

In the PBE simulation unphysical effects like the bridge-like shape of PTCDA and the rotation of the DATP central ring are present, which are amended when including vdW corrections (see Figure S8).

Finally, concerning the STM simulations described in the main text, we show in Figure S9 the theoretical image within the Tersoff-Hamann approximation for V_{bias}=+0.5 V.

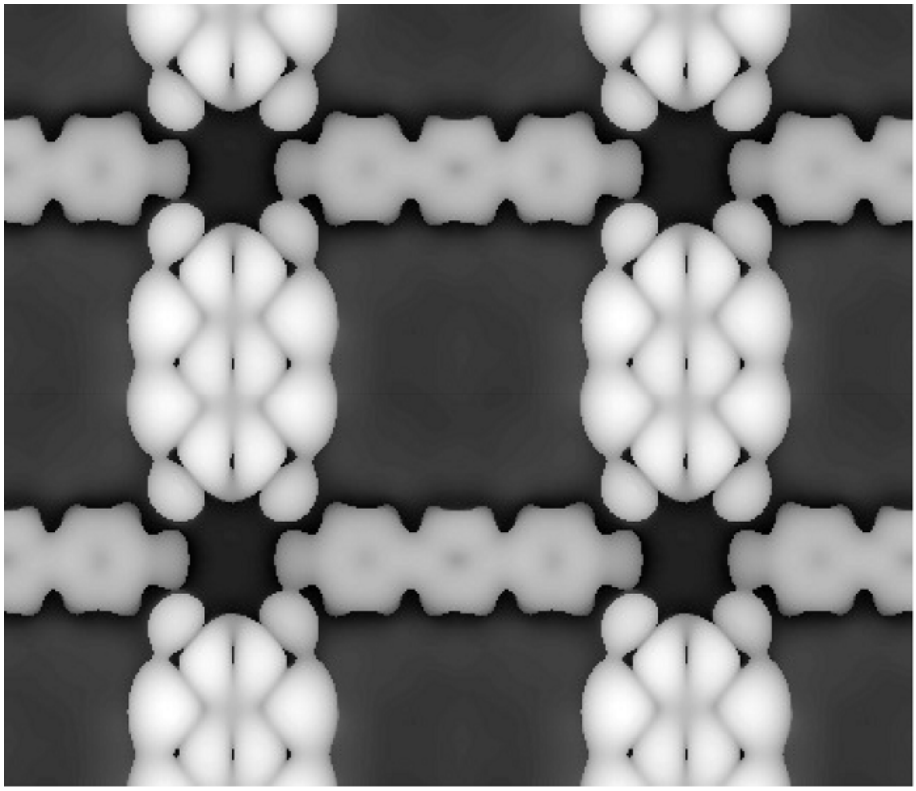

Figure S9. Simulated STM image at a bias of +0.5 V, without Gaussian smearing.

The shape of the LUMO from the gas-phase PTCDA is evident and correspond to the experimental observation that such features are conserved also in the adsorbed supramolecular phase.

As a support for Fig. 3 of the main manuscript, we report in Table S2 the geometrical parameters (width, peak height) for all biases, and we note again the overall very good correspondence between theory at the PBE-D level and experiment.

Bias (V)	**Experiment**		**PBE**		**PBE–D**	
	P/D width	**P/D height**	**P/D width**	**P/D height**	**P/D width**	**P/D height**
–1.8	1.31	1.23	0.85	0.91	1.34	1.24
–1.0	1.36	1.42	0.82	0.90	1.33	1.30
+0.2	1.51	1.93	1.71	2.16	1.66	1.75
+0.5	1.72	1.24	1.62	1.85	1.69	1.80

Table S2. Comparison between experimental and computed STM images at different biases (see Fig. 3 in the main manuscript). The ratios between the signal for PTCDA (P) and for DATP (D) are shown both for the full width at half maximum (P/D width)and for the height (P/D height)of the topography profiles.

References:

[S1] P. Fenter, F. Schreiber and L. Zhou, *Phys. Rev. B* **56** (1997) 3046.

[S2] T. Schmitz-Hübsch, T. Fritz, F. Sellam, R. Staub, and K. Leo, *Phys. Rev. B* **55** (1997) 7972.

[S3] M. Treier, M. T. Nguyen, N. V. Richardson, C. A. Pignedoli, D. Passerone, and R. Fasel, Nano Lett. 9, 126 (2009).

Table S3. Coordinates of PBE-D optimized PTCDA–DATP network on Au(111), surface unit cell 20.62469×17.86152 Å^2

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    314
Coordinate
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