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*Supporting Information to*

# "Inverted" Porphyrins: a Distorted Adsorption Geometry of Free-base Porphyrins on Cu(111)

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## Contents:

## *Computational procedures and details*

Periodic density functional theory calculations of 2H-TPP adsorbed on Cu(111) were performed with the Vienna Ab Initio Simulation Package (VASP)[1]. In general, the PBE functional[2] was used in combination with the third-generation van der Waals dispersion correction due to Grimme (DFT-D3)[3] and the projector-augmented wave (PAW) ansatz for the atomic cores[4, 5]. A plane-wave cutoff energy of 400 eV was employed. Van der Waals dispersion interactions play an important role for the adsorption of the 2H-TPP molecule to the copper surface. To check the sensitivity of the results on the description of van der Waals interactions, selected structures were also treated with other dispersion correction models, namely the 2009 dispersion correction due to Tkatchenko and Scheffler (DFT-TS)[6], the more sophisticated self-consistent screening van der Waals dispersion correction presented by the same authors (TS+SCS)[7], and the nonlocal optB86b-vdW method[8]. A good qualitative agreement was found for all van der Waals dispersion correction models, see the next section for details.

The Cu(111) surface was modeled as a 4-layer 9×10 slab (360 Cu atoms in total), where only the topmost two layers were freely optimized together with the adsorbed molecule, while the bottom two Cu layers were kept frozen at their optimized bulk positions. A vacuum layer of at least 10 Å was introduced to isolate the repeated slabs from each other. In a prescreening process for possible local minima, geometry optimizations from several starting geometries were done at the $\Gamma$ point in k-space only. For the final geometry optimizations of selected low-energy structures, a 2×2×1 Monkhorst-Pack (MP) k-point mesh was used. Geometries were optimized until the forces on the active atoms dropped below 0.01 eV/Å.

Numerical vibrational frequency calculations were performed for two of the optimized structures, i.e., the conventional saddle and the lowest-energy inverted adsorption geometries, using a slightly simplified slab model to verify the structures as local minima on the energy hypersurface. These numerical frequency calculations were performed on a three-layer Cu slab with all Cu positions frozen, and the $\Gamma$ point only was used. The structures had previously been optimized with the same 3-layer slab. No imaginary frequencies were found in these calculations, thus reassuring the structures as a true minimum. This also strongly suggests that the final geometries, which were subsequently refined with the full 4-layer slab described above, will also likely correspond to true local minima.

Scanning tunneling microscopy (STM) simulations were performed with the p4vasp program based on the Tersoff-Hamann model.[9, 10] N 1s core electron binding energy shifts (XPS shifts)[11] were estimated using VASP within the half-core hole (Slater transition state) approximation to the final state shifts using the $\Gamma$ point only and the optimized structures.

## *Comparison of structural data obtained from different dispersion corrections*

The Table S1 shows a comparison of salient structural parameters obtained from DFT-PBE calculations with the four different dispersion correction models used in this work, along with the experimental XSW data by Bürker et al.[12] (see Table 1 of the main text for corresponding PBE-D3 data only). Only data for the lowest energy orientations (which coincide with the orientations suggested by the STM experiments) are shown. The data shows that the distances to the surface differ by up to about 0.2 Å among the various dispersion correction models. However, all dispersion correction models consistently show a significantly better agreement of the inverted adsorption structure with experiment than the conventional saddle-shape structure. The inverted structure is thus confirmed by the present DFT-PBE calculations, independent of the dispersion correction model used. Hence, subsequently, as well as in the main text, all data refer to the PBE-D3 method only.

**Table S1.** Comparison of van der Waals correction schemes. Structural data on salient adsorption models optimized using the PBE functional and various vdW correction schemes in comparison to experimental data from XSW measurements[12]; average distances along the surface normal of specified atom groups to the average of the topmost layer of the Cu(111) slab in Å.

| Type | Method[a] | N (all) | =N- (iminic) | >NH (aminic) | C (all) | C (36)[b] |
|---|---|---|---|---|---|---|
| "saddle" (NH along <-110>) | **PBE-D3 / 2x2x1** | 2.990 | 2.993 | 2.988 | 3.240 | 3.140 |
| | PBE-TS / 2x2x1 | 3.056 | 3.076 | 3.036 | 3.291 | 3.181 |
| | PBE-oB86b / 2x2x1 | 2.964 | 2.983 | 2.945 | 3.301 | 3.204 |
| | PBE-SCS-TS / Γ | 3.038 | 3.040 | 3.037 | 3.306 | 3.228 |
| "inverted" (NH along <1-21>, N over bridge sites) | **PBE-D3 / 2x2x1** | 2.110 | 1.891 | 2.328 | 2.586 | 2.410 |
| | PBE-TS / 2x2x1 | 2.124 | 1.884 | 2.365 | 2.614 | 2.446 |
| | PBE-optB86b / 2x2x1 | 2.020 | 1.843 | 2.196 | 2.502 | 2.319 |
| | PBE-SCS-TS / Γ | 2.002 | 1.887 | 2.118 | 2.526 | 2.354 |
| Exp. | **XSW**[12] | **2.04 ± 0.06** | **1.97 ± 0.08** | **2.28 ± 0.05** | **2.34 ± 0.02** | |

a: Method and MP k-point mesh; b: C(36): considering only the 36 carbon atoms in the molecular plane; this value thus corresponds to the distance of the molecular plane to the substrate and neglects the 8 carbon atoms in the upright pyrrole rings; notably, the XSW experiment averages over all 44 carbon atoms.

## *Structural details on adsorption models of 2H-TPP on Cu(111)*

In Table S2 DFT-computed structural data for various orientations of the saddle and inverted structures are collected and compared to experimental XSW data. For each adsorption mode (saddle or inverted), two different orientations of the molecule with respect to the underlying Cu lattice were tested. The two orientations differ by a rotation of the adsorbed molecule by 90° around the [111] surface normal. In one orientation the imaginary line connecting the two NH groups of the molecule is parallel to a main crystallographic <-110> axis of the Cu 2D lattice, while in the other orientation this line is perpendicular to a main axis of the Cu(111) lattice. In each orientation, the adsorbate structure was fully optimized as specified in the Computational Details section. For the conventional saddle adsorption mode, we find only a very small energy difference (less than 0.2 eV) between the two orientations, which is below the expected accuracy of the computational method. A larger energy difference of 1.1 eV is obtained between the two orientations for the inverted adsorption mode (iminic N atoms over bridge sites, see below), giving favor to the orientation where the line defined by the two aminic NH groups is parallel to a main axis of the Cu(111) lattice.

For the saddle-shape adsorption mode, we also considered structures where the molecule is flipped over compared to the conventional saddle (labeled “upside-down saddle” in Table S2), i.e., where the NH groups are inclined towards the surface and the lone pairs of the iminic N atoms point away from the surface, again in two orientations defined by 90° rotation around the surface normal. One of these structures is found to have a slightly lower energy (by 0.2 eV) than the conventional saddle structures, which is, however, still higher than the energy obtained for the lowest-energy inverted structure by 0.3 eV. In addition, these alternative “upside-down” saddle-shape structures, which to our knowledge have not been considered before, do not agree with the experimental reference data, just as the conventional saddle structure. Hence, we do not consider these upside-down saddle-shape structures any further here. Instead, in the main text, we compare the inverted structure in comparison to the conventional saddle structure as a reference.

For the inverted structures, the question about the adsorption sites of the two iminic nitrogen atoms pointing “down” to the surface arises. We found stationary points in the geometry optimizations for inverted structures with the iminic nitrogen atoms and their lone pairs over top sites and over bridge sites, the latter being lower in energy by 0.7 eV than the former. In addition, the structural match of the “bridge-site” structure is in much better agreement with the experimental XSW data. We note that the energy difference between the atop and bridge structure (0.7 eV) coincides with the energy barrier of diffusion found of 2H-TPP on Cu(111) in experiments as reported in [13], suggesting that the lateral diffusion path of 2H-TPP on Cu(111) may resemble a hopping path between atop and bridge-site structures. The calculated energy profile along a linear interpolation of the atop and bridge-site structure, as well as the energy changes upon small displacements of the porphyrin molecule perpendicular to this path, indicate that the atop structure is a very shallow energy minimum and basically represents the saddle-point configuration for diffusion along the densely-packed Cu rows.

The present DFT calculations thus predict that the lowest-energy inverted structure is slightly lower in energy that any of the saddle-shape structures (neglecting free energy contributions). In general,

however, we consider the computed energy differences too small for a firm assignment of the favored adsorption mode on energetic grounds alone, although the relative energy ordering for the different orientations obtained is fully consistent with experimental observations. More stringent evidence comes from a comparison of the computed and measured STM and XPS data along with structural data, as discussed in the main text and below.

**Table S2.** Comparison of different adsorption models at the PBE-D3 level and experimental XSW data[12]; average distances along the surface normal of specified atom groups to the average of the topmost layer of the Cu(111) slab in Å; ΔE: relative energies of the various orientations / adsorption modes at 0K (PBE-D3); lowest energy structure within the conventional saddle, the upside-down saddle, and the inverted models are given in boldface.

| Type | Orientation / Adsorption mode | N (all) | =N- (iminic) | >NH (aminic) | C (all) | C (36)[a] | ΔE [eV] |
|---|---|---|---|---|---|---|---|
| "saddle" | **NH along <-101>** | **2.990** | **2.993** | **2.988** | **3.240** | **3.140** | **+0.55** |
| | NH along <1-21> | 2.970 | 2.980 | 2.960 | 3.222 | 3.116 | +0.56 |
| | Upside-down saddle<br>NH along <1-21> | **3.009** | **3.091** | **2.927** | **3.193** | **3.093** | **+0.34** |
| | Upside-down saddle<br>NH along <-101> | 3.130 | 3.208 | 3.051 | 3.274 | 3.167 | +0.51 |
| "inverted" | **NH along <1-21>, N near bridge sites** | **2.110** | **1.891** | **2.328** | **2.586** | **2.410** | **0.0** |
| | NH along <1-21>, N atop | 2.494 | 2.234 | 2.754 | 2.768 | 2.559 | +0.70 |
| | NH along <-101>, N near bridge sites | 2.245 | 2.062 | 2.429 | 2.678 | 2.504 | +1.09 |
| | NH along <-101>, N atop | 2.443 | 2.167 | 2.719 | 2.763 | 2.563 | +0.65 |
| Exp. | **XSW**[12] | **2.04 ± 0.06** | **1.97 ± 0.08** | **2.28 ± 0.05** | **2.34 ± 0.02** | | --- |

a: C(36): considering only the 36 carbon atoms in the molecular plane; this value thus corresponds to the distance of the molecular plane to the substrate and neglects the 8 carbon atoms in the upright pyrrole rings; notably, the XSW experiment averages over all 44 carbon atoms.

Figure S1 shows an alternative view of the lowest-energy adsorption structures “from the bottom”, i.e., seen through the top Cu layer (deeper Cu layers are not shown). Cf. Figure 1 of the main text.

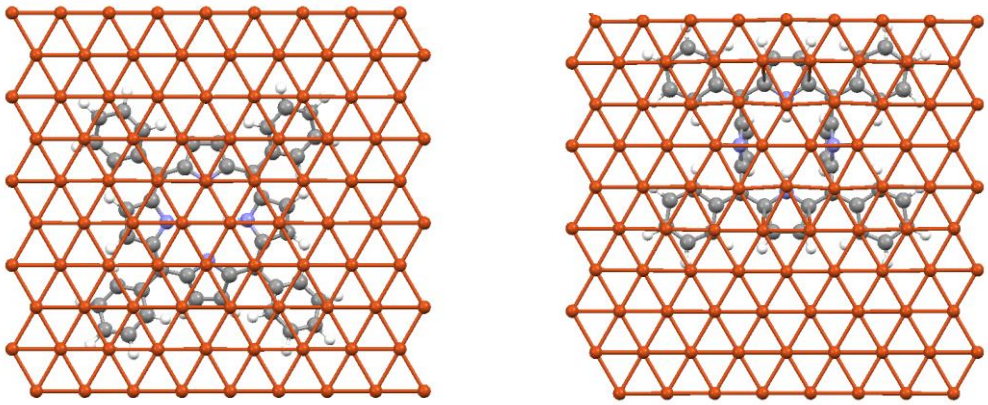


**Figure S1.** Illustration of the lowest-energy saddle-shape (left) and inverted (right) adsorption structures of 2H-TPP on Cu(111) in relation to the Cu atoms in the top layer of the surface slab from the present DFT calculations, cf. also Figure 1 of the main paper for alternative representations of the same structures; view from the Cu slab “through” the top Cu(111) layer to the molecule; color code: Cu copper, N blue, C grey, H white.

## *Adsorption energies from DFT calculations*

**Table S3.** Adsorption energies in eV of 2H-TPP on Cu(111) in the lowest-energy geometries found in the present DFT calculations with the PBE functional and various vdW correction schemes; [eV]; 2x2x1 k-point mesh.

| **vdW method** | **saddle** | **inverted** |
|---|---|---|
| D3 | 4.76 | 5.31 |
| TS | 6.78 | 7.13 |
| oB86b | 3.89 | 4.81 |
| SCS-TS[a] | 5.60 | 6.30 |

a: For SCS-TS, geometries were optimized using the $\Gamma$ point only.

## *Core level photoelectron spectroscopy: N 1s splittings*

Table S4 shows the calculated differences in N 1s core level binding energies between the aminic (>NH) and iminic (=N-) nitrogen atoms of 2H-TPP on Cu(111) in the lowest-energy geometries found for each configuration, in comparison to corresponding experimental XPS data.

**Table S4.** N 1s core level binding energy splittings of iminic vs. aminic nitrogen atoms calculated using the DFT-PBE and the Slater-transition-state method[11], i.e., including approximate final state effects, versus experiment; in eV.

| **Configuration** | **adsorbed on Cu(111) / monolayer** | **free molecule / multilayer[a]** |
|---|---|---|
| Saddle | 2.2 | 2.2 eV |
| Upside-down saddle[b] | 1.9 / 2.0[c] | |
| Inverted | 1.4 | |
| Experiment[d] | 1.5 / 1.6 | 2 eV |

a: gas phase geometry in large box ($35^3$ Å$^3$), description as “saddle” or “inverted” does not apply for the gas phase geometry; b: 2H-TPP adsorbed “upside down” compared to conventional saddle geometry: both >NH inclined towards surface, =N- lone pairs inclined away from surface; c: values for geometries with molecules rotated 90° around the surface normal; d: experimental monolayer and multilayer data from [14,15].

## *Interfacial charge rearrangement upon adsorption*

In this section we compare the charge rearrangement at the interface upon adsorption from the present DFT (PBE-D3) calculations for the lowest-energy conventional saddle-shape structure and the new inverted adsorption geometry. The calculated charge (Bader partitioning scheme) on the 2H-TPP molecule is -1.91 e for the inverted geometry, but only -0.08 e for the conventional saddle geometry, i.e. electron charge is transferred from the surface to the molecule upon adsorption. Note that the amount of charge transferred is much larger for the inverted structure than for the saddle geometry.

In Figure S2 we compare calculated charge density difference (CDD) plots for both adsorption geometries using the same contour value. For the inverted structure, the map shows a loss of electron density (magenta in Figure S2) on the molecule in the region where the nitrogen lone pairs bind to the surface, which is indicative of a dative bond of the molecule to the surface. The two binding N also gain some charge close to the N centers, but not in the lone pair region. On the other hand, the molecule gains electron charge (green areas in Figure S2) in its $\pi$ system, especially at the meso C atoms (where the phenyl rings are attached to), and in the phenyl rings (the two ortho-C and the para C). The two backside C atoms (2,3) of the parallel pyrrole rings also significantly gain electron charge. Interestingly, also the two side bonds of the upright pyrrole rings (i.e., the bonds between the 1,2 and 3,4 C atoms locally gain electron density.

As can also be seen from Figure S2, much less charge is rearranged upon adsorption for the conventional saddle, in agreement with the low amount of charge transfer stated above. To show more detail here, additional CDD plots with lower contour values are shown in Figure S3.

Rojas et al. measured the local work function at the adsorption site, indicating a drop in work function over the central part of the molecule and an increase over the peripheral phenyl rings, compared to bare Cu(111). [16] This seems to compare well with our CDD map of the inverted structure, Figure S2, at least qualitatively. In the same paper, Rojas et al. also show a calculated CDD map based on a conventional saddle structure adsorbed on a finite metal cluster and a small contour isodensity value, which compares well with our corresponding data in Figure S3.

In summary, our CDD map for the inverted structure appears compatible with the experimental observations of Rojas et al.: charge-transfer from the surface to the peripheral phenyl rings (leading to a local increase of surface dipole and therefore also increase in the local work function), while the "upright" pyrrole rings lose electron density to the surface via donation by the nitrogen lone pairs (compatible with a local work function decrease). Hence, electron donation occurs from the molecule to the surface via the coordinating N atoms, while the flat-lying peripheral phenyl rings act as electron acceptors. Our CDD map for the inverted structure thus confirms the donor-acceptor model discussed for 2H-TPP adsorption in a more consistent way that the conventionally assumed saddle geometry.

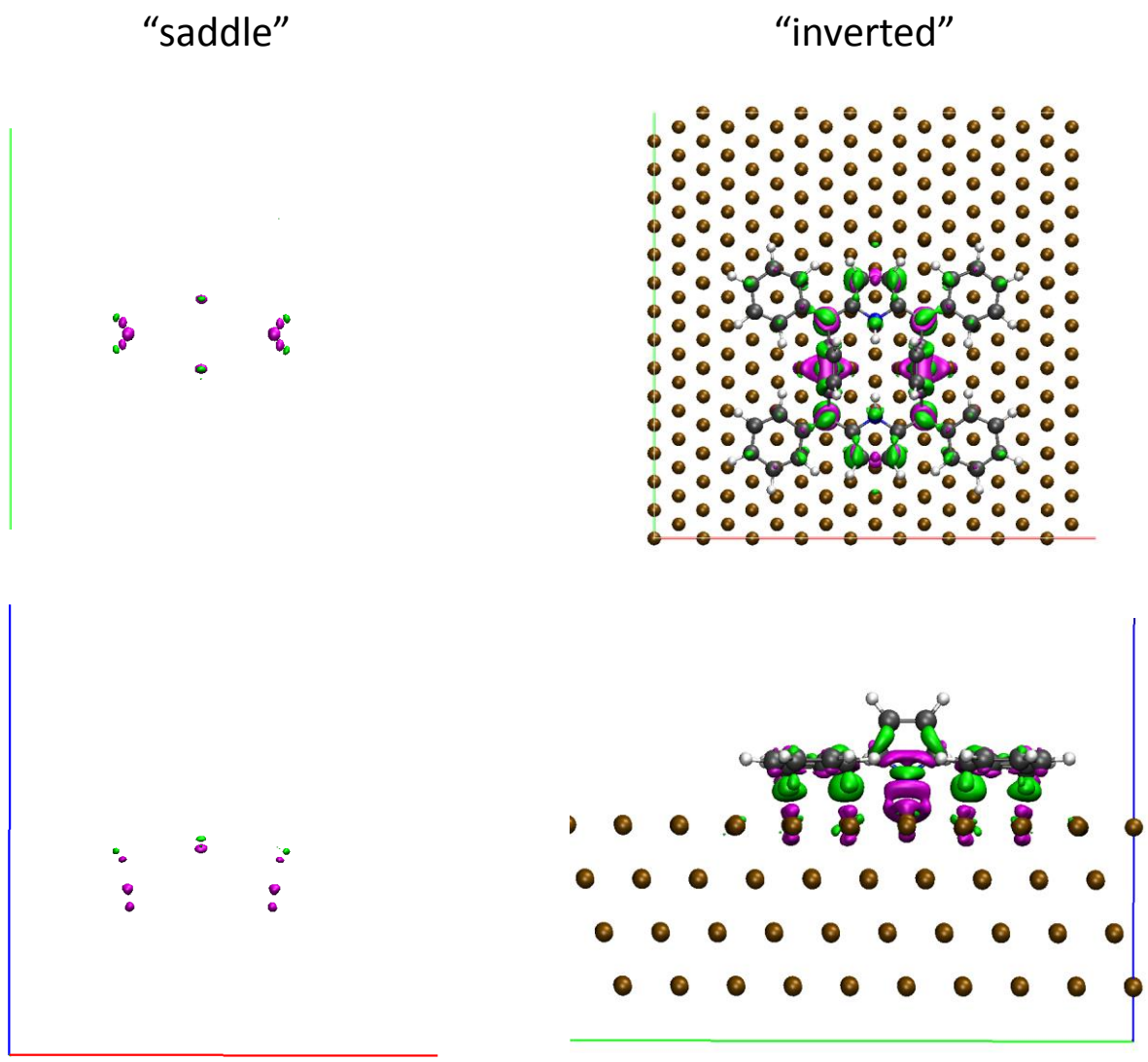
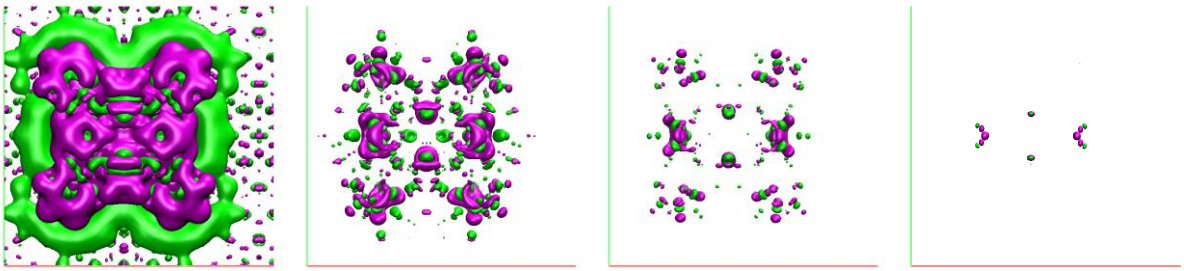



**Figure S2.** Calculated charge-density difference contours for 2H-TPP on Cu(111) in the saddle-shape (left) and inverted (right) adsorption geometry; green: local gain of electron density, magenta: local loss of electron density compared to the isolated molecule / surface with fixed geometry; contour: 0.03 e/Å$^3$. The degree of interfacial charge transfer is much smaller in the saddle-shape structure than in the inverted structure. Atomic symbols were omitted in the left panels for better visibility; see Figure S3 for additional choices of isodensity values for the saddle-shape structure.



0.001 0.005 0.01 0.03

**Figure S3.** Calculated charge-density difference contours for 2H-TPP on Cu(111) in the saddle-shape adsorption geometry with different contour values, top view; green: local gain of electron density, magenta: local loss of electron density compared to the isolated molecule / surface with fixed geometry. The rightmost image corresponds to the same isodensity value (0.03 e/Å$^3$) as in Figure S2.

## *Cyano-functionalized 2H-TPP on Cu(111)*

The periodic DFT calculations for the free-base cyano-functionalized 5,10,15,20-tetrakis(para-cyano phenyl) porphyrin (2H-TCNPP) on the Cu(111) surface were done with a slightly different computational setup. The PWscf code of the Quantum Espresso software package[17] was used together with Vanderbilt ultrasoft pseudopotentials[18] and a plane-wave cutoff energy of 30 Ry. However, the same density functional (PBE)[2] and the same van der Waals dispersion correction scheme (Grimme-D3)[3] as in the calculations for 2H-TPP were employed.

The Cu(111) surface was represented by a 3-layer slab with lateral size of (10×10) surface unit cells (300 Cu atoms in total). The two topmost layers together with the adsorbed molecule were relaxed using a force convergence threshold of 0.003 eV/Å, while the bottom Cu layer was kept frozen. As in the 2H-TPP calculations, the $\Gamma$ point approximation was used for a prescreening of possible local minimum structures, but all final results are reported for a 2×2×1 Monkhorst-Pack k-point mesh.

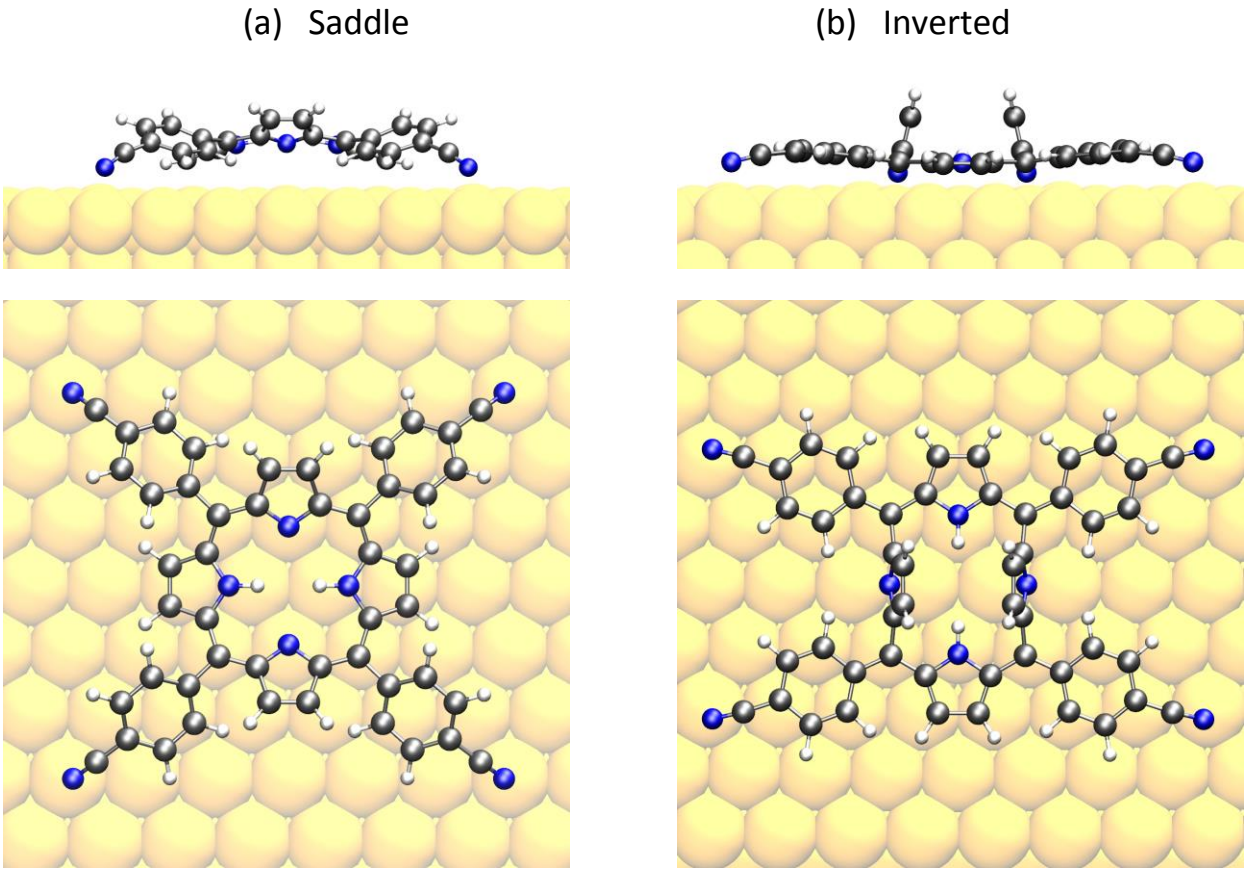



**Figure S4.** Top and side views of the optimized geometries of 2H-TCNPP on Cu(111). (a) Conventional saddle-shape and (b) inverted adsorption configuration.

Eight different configurations of adsorbed 2H-TCNPP molecules were considered in the DFT calculations: the conventional saddle-shape, the upside-down saddle-shape and the inverted configuration, all of them with the NH…HN axis either oriented parallel or perpendicular to the close-packed <$\bar{1}10$> Cu rows. In addition, two different lateral positions were considered for the most favorable orientation of the conventional saddle-shape and the inverted configuration: the iminic nitrogens were either ontop of a surface Cu atom or in a bridging position between two Cu atoms.

As for the 2H-TPP molecules, we also find for the cyano-functionalized porphyrins that the inverted configuration with an orientation of the NH…HN axis perpendicular to the <$\bar{1}10$> Cu rows and the iminic nitrogens in a bridging position is the global energy minimum. This structure is more stable by a small margin of about 0.6 eV than the conventional saddle geometry in its most favorable orientation, which is rotated by 90° compared to the inverted configuration (see Figure S4). The structure of the porphyrin core of the 2H-TCNPP molecules is quite similar as in the case without cyano-functionalization of the phenyl rings (compare Figure S4 with Figure 1 in the manuscript). The phenyl rings, however, show different orientations since the CN groups have a strong preference to sit on top of a surface Cu atom. In the saddle-shape geometry the bending-down of the CN groups leads to an overall bending of the 2H-TCNPP molecule, which slightly lifts the porphyrin core from the surface: the average height of the N atoms above the surface increases from 2.98 Å for 2H-TPP (see Table S2) to 3.20 Å for 2H-TCNPP. In the inverted configuration the interaction of the CN groups with the Cu surface atoms results in a strong elongation of the 2H-TCNPP molecule and an even more pronounced rectangular shape.

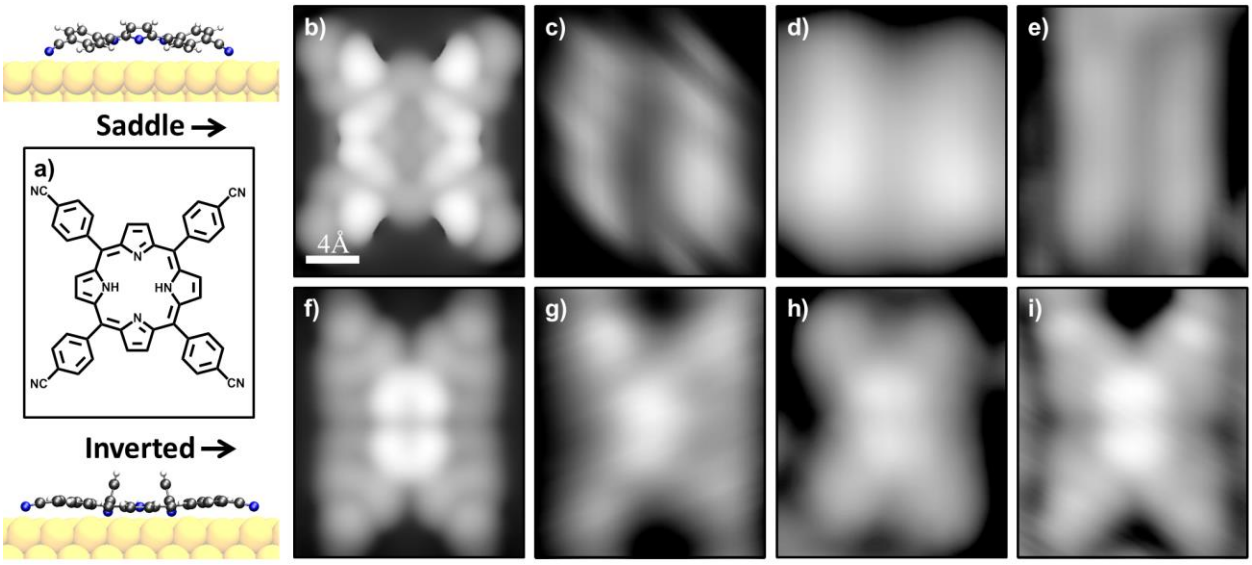



**Figure S5.** (a) Chemical structure of 2H-TCNPP. Simulated STM data (V = -1.0 V, isodensity contour = $10^{-6}$ e/bohr$^3$) are shown in (b) for the saddle-shape and in (f) for the inverted structure. (c-e) Experimental STM data of the two protrusion appearance measured in Erlangen at RT (V = -1.0 V, I = 27 pA) (c) and at LT (V = 1.0 V, I = 0.2 nA) (d), as well as at RT in Campinas (V = -1.7 V, I = 0.25 nA) (e). Similarly (g-i) show experimental STM data of the inverted structure appearance measured in Erlangen at RT (V = -1.2 V, I = 26 pA) (g) and at LT (V = 0.5 V, I = 0.1 nA) (h) as well as at RT in Campinas (V = -1.4 V, I = 0.18 nA) (i).

STM images for the two configurations of Figure S4 were calculated in the Tersoff-Hamann approximation[9, 10] using our own post-processing code[19]. They are shown in Figure S5 together with three sets of measured STM images, taken independently from each other in three different vacuum chambers. As for 2H-TPP, also two different appearances are observed for the 2H-TCNPP molecules. The elongated, rectangular shape of the 2H-TCNPP molecules in the measured images, however, can only be explained by the inverted configuration but not the saddle-shape geometry.

Finally we also report the differences in the N 1s core electron binding energy between the aminic (>NH) and iminic (=N-) nitrogen atom in Table S5, although no experimental data is available for 2H-TCNPP on Cu(111). The splittings were calculated by two methods: the half-core hole (Slater transition state) approximation and by ΔSCF calculations. For the Slater transition state calculations a new nitrogen pseudopotential was constructed from an atomic configuration with a half core hole, and the N 1s level was included in the pseudopotential as a valence state. This pseudopotential was then successively used for one of the four phorphyrin nitrogen atoms in four separate SCF calculations (again, the N 1s level was only occupied by ½ electron). The supercell was made charge-neutral by a compensating homogeneous background charge. The XPS splitting is then given by the difference of the N 1s eigenvalues. The ΔSCF calculations were done in a similar way, however, using a different nitrogen pseudopotential, constructed from an atomic configuration with a full core hole without including the N 1s level as valence state, and the XPS splitting is then determined from the total energy difference. In this case, the supercell was made charge neutral by adding one electron to the valence states at the Fermi energy. The results in Table S5 show that the CN-functionalization of the phorphyrin molecules has no significant effect on the XPS core level splittings and the same structure-dependence as for 2H-TPP is seen.

**Table S5.** N 1s core electron binding energy splittings (in eV) of iminic vs. aminic nitrogen atoms for 2H-TCNPP adsorbed on Cu(111), calculated either by the Slater-transition-state or the ΔSCF method. The corresponding values for the 2H-TCNPP gas phase molecule are 2.16 eV (Slater) and 2.16 eV (ΔSCF).

| **Configuration** | **Slater** | **ΔSCF** |
|---|---|---|
| Saddle, NH along <$\bar{1}10$> | **2.24** | **2.23** |
| Saddle, NH along <$1\bar{2}1$> | 2.11 | 2.11 |
| Upside-down, NH along <$\bar{1}10$> | 2.17 | 2.18 |
| Upside-down, NH along <$1\bar{2}1$> | 1.93 | 1.96 |
| Inverted, NH along <$\bar{1}10$> | 1.82 | 1.79 |
| Inverted, NH along <$1\bar{2}1$> | **1.38** | **1.33** |

## *Experimental section – Erlangen*

The experiments and sample preparations were performed in two different ultrahigh vacuum (UHV) systems at a background pressure in the low $10^{-10}$ mbar regime. One of the experimental setups houses a variable temperature scanning tunneling microscope (STM), namely a RHK UHV VT STM 300 operated at RT with a RHK SPM 1000 electronics. The images taken at 80 K where obtained with a homebuilt LT-STM. All STM images were acquired in constant current mode with a Pt/Ir tip (RT-STM) or etched W tip (LT-STM) with the bias voltage applied to the sample. The STM images were processed with WSxM software and moderate filtering (Gaussian smoothing, background subtraction) was applied for noise reduction[20]. The preparation of the clean Cu(111) surface was done by repeated cycles of $Ar^+$ sputtering (500 eV) and annealing to 850 K. The 5,10,15,20-tetraphenyl porphyrin (2H-TPP) and the 5,10,15,20-tetrakis(para-cyanophenyl) porphyrin (2H-TCNPP) molecules were deposited onto the metal substrates held at RT, by thermal sublimation from a home-built Knudsen cell at 300°C and 340°C, respectively. The ⟨110⟩ axes of Cu(111) were either determined directly by the imaging of the Cu dense-packed rows at LT or by co-deposition of 2H-TPP on Cu(111) which azimuthal orientation is known to coincide with the crystallographic main directions of Cu(111) at RT.

## *Experimental section – Campinas*

All experiments were performed in two connected ultra-high vacuum (UHV) chambers. One chamber was equipped with a STM and the other one with standard cleaning facilities, XPS and home-made Knudsen cells for molecule sublimation. The pressure in the XPS chamber was in the low $10^{-10}$ mbar range and in the STM in the middle $10^{-11}$ mbar range. The STM microscope used was a SPECS Aarhus 150 equipped with a SPECS SPC 260 Controller. The STM measurements were performed in constant current mode with a W tip cleaned in situ by $Ar^+$ sputtering. All STM images were taken at room temperature (RT), plane-corrected and Gaussian smoothed with WSxM[20]. The photons used in XPS were provided by a Al-Kα anode and the photoelectrons were analyzed with a SPECS Phoibos 150 hemispherical analyzer with multi channeltron detection. The Cu(111) crystal was prepared with repeated cycles of sputtering with $Ar^+$ ions (1 keV) and annealing (850 K) in UHV. 2H-TPP and 2H-TCNPP were deposited using two home-made Knudsen cell from quartz-crucibles heated to 300°C and 350°C, respectively.

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## *Atomic coordinates of optimized geometries*

PBE-D3 level, see the "Computational procedures" section and the main paper for details; VASP POSCAR format.

*Inverted geometry of 2H-TPP on Cu(111), NH groups along* $\langle 1\bar{2}0 \rangle$ *directions, N near bridge sites.*

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C H N Cu
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Selective
Cartesian
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*Saddle shape geometry, NH along* $\langle\bar{1}01\rangle$ *directions.*

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C H N Cu
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Selective
Cartesian
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