

Supplemental Material to Adsorption structures and energetics of molecules on metal surfaces: bridging experiment and theory

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I. COMPUTATIONAL DETAILS

A. Rare-Gas Adsorption on Metal Surfaces

We performed PBE+vdW^{surf} structure optimizations for Xe on five transition metal surfaces. The DFT calculations were performed using the all-electron/full-potential electronic structure code FHI-AIMS which uses numerical atomic-orbitals (NAO) as basis set^{1,2}. This code provides a hierarchy of predefined settings which give access to basis set levels and other settings at which fast relaxations can be safely performed. For all calculations of this section, we used *tight* settings, which include the *tier 1* standard basis set for the transition metals and Xe. The convergence criteria in the calculations were 10^{-5} electrons for the electron density and 10^{-6} eV for the total energy of the system. For all structure relaxations, $0.01 \text{ eV}\text{\AA}^{-1}$ was established as convergence criterion for the maximum final force. Relativistic effects were included via the atomic scalar zeroth-order regular approximation^{3,4}. We used the repeated-slab method to model all the systems together with the PBE xc functional⁵. We have used the PBE optimized lattice constant to generate the metal slabs: 4.149, 3.631, 3.971, and 3.943 \AA for Ag, Cu, Pt, and Pd, respectively⁶.

For the adsorption structure of the systems, we adopted the experimentally reported $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure with top and fcc-hollow adsorption sites for the (111) surface of Pt, Pd, and Cu. For the case of the Cu(110) surface, we present the results for a 2×2 surface unit cell. We used a Monkhorst-Pack⁷ grid of $15 \times 15 \times 1$ k-points in the reciprocal space and six metallic layers to perform the calculations, except for Cu(110), where we used seven metallic layers. The width of the vacuum gap was 20 \AA . For the relaxation of the systems, the Xe atom and the atoms in the topmost and first subsurface layers of the surface slab were allowed to relax. As we generated the substrates using the PBE lattice constant, we did not consider vdW interactions between metal atoms in order to avoid an artificial relaxation of the surfaces.

The vdW interactions were taken into consideration only in final adsorption energy calculations. The adsorption energies were computed using

$$E_{\text{ad}} = E_{\text{AdSys}} - (E_{\text{Me}} + E_{\text{Xe}}), \quad (1)$$

where E_{AdSys} is the total energy of the adsorption system (gas + metal surface) after relaxation, E_{Me} is the energy of the bare slab after relaxation, and E_{Xe} is the energy of the isolated Xe gas atom.

B. Aromatic Molecules Adsorbed to Metal Surfaces

1. Benzene on Cu(111), Au(111), and Pt(111)

The DFT calculations for benzene on coinage metal surfaces employed the numeric atom-centered basis set all-electron code FHI-AIMS^{1,2}. We employ the vdW-inclusive PBE+vdW^{surf} approach⁸ to account for vdW interactions and collective response effects. The scaled zeroth-order regular approximation⁹ was applied for treating relativistic effects. The *tight* settings including the *tier 2* standard basis set were used for H and C, and *tier 1* for transition metals. A convergence criterion of $10^{-2} \text{ eV}\cdot\text{\AA}^{-1}$ for the maximum final force was used for structural relaxations. Also, convergence criteria of 10^{-5} electrons per unit volume for the charge density and 10^{-4} eV for the total energy of the system were utilized for all computations. Adopting these settings, the numerical accuracies in determining the binding energy and equilibrium distance are better than 0.01 eV and 0.01 \AA , respectively.

2. Naphthalene on Cu(111), Au(111), and Pt(111)

The substrates were created using the lattice parameters for Cu, Au and Pt obtained with PBE+vdW^{surf} and contained in Ref. 6. The unit cells were created having dimensions (3×3) and six layers. The axis $Z = 35 \text{ \AA}$ includes the substrate, the monolayer and the vacuum. A naphthalene molecule per cell was positioned at an initial distance of 2.00 \AA above the top layer and 8 configurations were formed: atop, hcp, fcc, and bri respectively

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with 0 and 30° rotation. Computational calculations were carried out using FHI-AIMS¹ and the following convergence criteria: total energy = 10⁻⁴ eV, force = 10⁻² eV/Å and electron density=10⁻⁵ electrons. The binding energies were obtained after 3 stages of calculation: the first consisted in using the top 3 layers of the substrate and the Np molecule, the two upper layers were set free to relax, while the bottom layer was kept fixed. The degree of theory of the basis functions corresponds to light and *tier 2* for all elements. In the second stage, three bottom layers were added, fixed in their initial positions and maintaining the same level of basis function theory. Finally, the three most stable systems were computed with *tight* setting, using *tier 1* for the metallic substrates and *tier 2* for the monolayer. The calculations were coupled with the zeroth-order regular approximation⁹ (ZORA) to include the relativistic effects. The binding energy is obtained from the total energy of the entire system (E_{AdSys}), surface (E_{Me}) and molecule (E_{Np}) using:

$$E_{\text{ad}} = E_{\text{AdSys}} - (E_{\text{Me}} + E_{\text{Np}}). \quad (2)$$

The adsorption heights correspond to the difference between the average positions of the C atoms and the top layer of the substrate.

C. Extended and Compacted Carbonsystems on Metal Surfaces

General calculation settings

All the calculations in this section were performed using the full-potential all-electron code FHI-AIMS¹. We used, as exchange-correlation functional, the DFT+vdW^{surf} functional⁸, coupled with PBE⁵. All the metal substrates are built using the lattice constants determined from the PBE+vdW^{surf} method⁶. Convergence criteria of 10⁻⁵ electrons for the electron density and 10⁻⁶ eV for the total energy were employed. The maximum final forces were converged with a criterion of 0.01 eV/Å. Relaxations have been performed with *light* settings, while the final cohesive energies are computed using the *tight* settings. In our calculations, the scalar relativistic effects were included via the scaled zeroth-order regular approximation⁹ (ZORA).

1. DIP on Cu(111), Ag(111) and Au(111)

For all the three metal surfaces, we considered a (7×7) unit cell composed by three metal layers and a single DIP molecule. We set a vacuum level of 60 Å and a Monkhorst-Pack⁷ grid of 4×2×1 k-points. The central ring of the molecule is placed above an atom of the topmost metal layer and the major axis of the molecule is aligned along the unit cell diagonal. First, we obtained the adsorption energy curve by considering a rigid

DIP molecule and tuning the surface–molecule distance d . The adsorption energy per molecule E_{ad} was calculated via the formula:

$$E_{\text{ad}} = E_{\text{AdSys}} - (E_{\text{Me}} + E_{\text{DIP}}), \quad (3)$$

where E_{AdSys} is the energy of the combined system, E_{Me} and E_{DIP} are the energies of the isolated metal surface and the DIP molecule respectively. As a next step, we considered the geometry with lowest E_{ad} for all the three systems and performed a relaxation. During the relaxation, the two lowest-lying metal layers are kept frozen in their initial coordinates, while the topmost layer and the molecule are allowed to relax.

For DIP/Ag(111), we employed also the two unit cells observed in STM and LEED experiments¹⁰. The first unit cell is a $\begin{pmatrix} 6 & 2 \\ 1 & 4 \end{pmatrix}$ surface with three metal layers and a single DIP molecule in a brick-wall arrangement. A k-point grid of 2×4×1 and a vacuum of 60 Å has been used for this structure. The second is a $\begin{pmatrix} 11 & 0 \\ 2 & 4 \end{pmatrix}$ unit cell with three metal layers and two DIP molecules in a herringbone superstructure. Here we used a k-point mesh of 1×3×1 and a vacuum of 60 Å. Finally, we considered a brick-wall arrangement for DIP/Au(111), following experimental evidence obtained with STM and LEED techniques¹¹. The two molecules are arranged in a (9×5) unit cell with three metal layers and a vacuum of 60 Å. The k-space is sampled with 2×3×1 points.

2. C₆₀ on Ag(111) and Au(111)

For these two systems, we considered a $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ unit cell with one C₆₀ molecule. This structure is observed in STM experiments^{12,13}, using both Ag(111) and Au(111) as metal substrate. The simulated unit cell contains six metal layers, a vacuum of 60 Å and a Monkhorst-Pack⁷ grid of 2×3×1 k-points. In the experimental structure, the molecule presents a hexagon face parallel to the surface, located with its center above a top atom. However, this particular top atom is absent. In our DFT calculations, we reproduced the observed configuration, as well as the presence of the vacancy. During the relaxation procedure, all the six metal layers were allowed to relax. In this way we could compare with the experiments, not only the distance between the topmost metal layer and the molecule, but also the interlayer spacing.

In order to compute the adsorption energy per molecule E_{ad} , we included the presence of a vacancy in the metal substrate with the formula:

$$E_{\text{ad}} = E_{\text{AdSys}} - (E_{\text{Me}} + E_{\text{C}_{60}} + E_{\text{Vac}}), \quad (4)$$

where the energy of the isolated substrate E_{Me} and the energy of the molecule $E_{\text{C}_{60}}$ are subtracted to the energy of the whole system E_{AdSys} . The last term, E_{Vac} , refers to the energy required to form a vacancy. This value depends on the metal substrate, in this work we used

$E_{\text{Vac}} = 0.67 \text{ eV}^{14}$ and 0.83 eV^{15} for Ag(111) and Au(111) respectively.

D. Sulfur-containing Systems on Metal Surfaces

DFT+vdW^{surf} calculations coupled with the PBE functional were performed employing the FHI-AIMS code with atom-centered orbitals (NAOs) basis set¹. To perform adsorption calculations, we created (4×3) super cells for Au, Ag and Cu (111) surfaces. The lattice parameters are taken from Ref. 6. The Z axis is set to 35 \AA and corresponds to the substrate plus vacuum. All three substrates are made with six metal layers, during the relaxation topmost two layers were free to move, while the bottom four layers remained fixed in their initial positions. The thiophene monolayers at low coverage were emulated with one molecule per unit cell. The molecule was placed at 2.00 \AA above the metallic substrates. We searched for a stable final binding distance and configuration, starting from 8 initial states: atop, hcp, fcc, and bri with 0 and 30 rotations. We employed the following convergence criteria: total energy = 10^{-4} eV , force = $10^{-2} \text{ eV/\AA}^{-1}$, electron density = 10^{-5} electrons and k space of $3 \times 3 \times 1$. We used *tight* setting in conjunction with *tier 2* for Ag, Au and Cu atoms combined with *tier 3* for C, S and H atoms. The atomic scalar zeroth-order regular approximation⁴ was employed to address relativistic effects. The adsorption energy is computed *via*:

$$E_{\text{ad}} = E_{\text{AdSys}} - (E_{\text{Me}} + E_{\text{Thp}}), \quad (5)$$

where E_{AdSys} correspond to the total energy of the entire system, E_{Me} is the total energy of the metallic surface and E_{Thp} the one of the isolated thiophene molecule.

E. Oxygen-containing systems on Metal Surfaces

1. General calculation settings

We present the general settings for the DFT calculations analyzed in this section, particular settings are mentioned below. All calculations were performed using the all-electron/full-potential electronic structure code FHI-AIMS¹. This section comprises calculations with both *light* and *tight* settings, where *light* settings include the *tier 1* NAO basis set for C, H, O, and the metal substrate; while *tight* settings include the *tier 1* NAO basis set for the metal substrate and the *tier 2* NAO basis set for C, H, and O. The convergence criteria were 10^{-5} electrons for the electron density and 10^{-6} eV for the total energy of the system in all calculations. For all structure relaxations, we used 0.01 eV\AA^{-1} as convergence criterion for the maximum final force. Relativistic effects were included via the atomic scalar zeroth-order regular approximation⁴. We used the repeated-slab method to model all the systems together with the PBE xc functional⁵.

2. PTCDA on Ag(111), Ag(100), and Ag(110)

PTCDA forms a commensurate monolayer structure on silver surfaces. The lateral ordering of the molecules in the monolayer depends on the orientation of the surface (see, for example, Ref. 16). The surface unit cells for the calculations were modeled with a $\begin{pmatrix} 6 & 1 \\ -3 & 5 \end{pmatrix}$, $\begin{pmatrix} 4 & 4 \\ -4 & 4 \end{pmatrix}$, and a $\begin{pmatrix} 3 & 2 \\ -3 & 2 \end{pmatrix}$ super cell for the case of Ag(111), Ag(100), and Ag(110), respectively, in accordance to experimental results^{17,18}. We generated all surface slabs with the PBE lattice constant of Ag, which is 4.149 \AA , in accordance with the work by Liu *et al.*⁶. The slabs consisted of five layers for Ag(111) and Ag(100) and seven layers for Ag(110) each with a vacuum gap of 50 \AA . We used a Monkhorst-Pack⁷ grid of $4 \times 4 \times 1$ for Ag(111) and $6 \times 6 \times 1$ k-points for Ag(100) and Ag(110) in the reciprocal space. We performed a structural relaxation of each of these systems where the molecule and the atoms in the topmost two metal layers were allowed to relax using the PBE+vdW^{surf} method taking the experimental configuration as starting point for each structural relaxation. We did not take into account vdW interactions between metal atoms in the structural relaxations in order to avoid an artificial relaxation of the surface due to the fact that the surface slab was created using the PBE lattice constant. They were taken into consideration only in final adsorption energy calculations. All calculations were performed using *tight* settings as described above.

Adsorption energies E_{ad} for PTCDA on Ag(111), Ag(100), and Ag(110) are calculated with the PBE+vdW^{surf} method using

$$E_{\text{ad}} = \frac{1}{N} (E_{\text{AdSys}} - E_{\text{Me}} - E_{\text{PTCDA}}), \quad (6)$$

where E_{AdSys} is the total energy of the adsorption system (PTCDA + metal surface), E_{Me} is the energy of the bare metal slab, E_{PTCDA} is the energy of the monolayer in periodic boundary conditions. N corresponds to the number of PTCDA molecules per unit cell, namely $N = 2$ for PTCDA on Ag(111) and Ag(100), while $N = 1$ in the case of Ag(110). All quantities are taken after relaxation of each subsystem.

3. PTCDA on Au(111)

PTCDA does not form commensurate monolayers on the Au(111) surface but rather exhibits a situation close to a point-on-line growth on the $(22 \times \sqrt{3})$ reconstructed surface, situation which is not accessible to any type of state-of-the-art modeling¹⁹⁻²². We generated the surface slab with the PBE lattice constant of Au, which is 4.159 \AA , in line with a previous investigation⁶. As a reasonable approximation (see Ref. 23), we have modeled the system using a $\begin{pmatrix} 6 & 1 \\ -3 & 1 \end{pmatrix}$ surface unit cell consisting of five layers each with thirty three Au atoms. The adsorbed monolayer consists of a herringbone lateral arrangement of two PTCDA molecules per unit cell. We

chose the size of the vacuum gap to be approximately 50 Å and a Monkhorst-Pack⁷ grid of $4 \times 4 \times 1$ k-points in the reciprocal space. We performed the structural relaxation of the system using the PBE+vdW^{surf} method by fixing the Au atoms in the three bottom layers. For the structural relaxations, we did not take into account vdW interactions between metal atoms in order to avoid an artificial relaxation of the surface due to the fact that the surface slab was created using the PBE lattice constant. They were taken into consideration only in the calculation of the final adsorption energies. All calculations were performed using *tight* settings as described above.

We have calculated the adsorption energy per molecule for two different coverages Θ of 1.0 and 0.5 ML with the PBE+vdW^{surf} method. In this model, $\Theta = 1.0$ ML corresponds to the adsorption of two PTCDA molecules per surface unit cell while $\Theta = 0.5$ ML corresponds to the adsorption of one molecule per surface unit cell. The adsorption energy per molecule was calculated using

$$E_{\text{ad}}^{\Theta(\text{ml})} = \frac{1}{N} [E_{\text{AdSys}}^{\Theta} - (E_{\text{Au}} + E_{\text{PTCDA}}^{\Theta})], \quad (7)$$

$$E_{\text{ad}}^{\Theta(\text{gas})} = \frac{1}{N} [E_{\text{AdSys}}^{\Theta} - (E_{\text{Au}} + N \cdot E_{\text{PTCDA}}^{\text{gas}})], \quad (8)$$

where $E_{\text{AdSys}}^{\Theta}$ is the energy of the complete system formed by the monolayer and the slab, E_{Au} is the energy of the slab and $E_{\text{PTCDA}}^{\Theta}$ is the energy of the monolayer in periodic boundary conditions. N corresponds to the number of molecules in the model of the system, $N = 2$ in the specific case of PTCDA/Au(111). Equation (7) does not consider the formation of the monolayer in its definition of adsorption energy, while Eq. (8) considers the formation of the monolayer from gas phase by using $E_{\text{PTCDA}}^{\text{gas}}$, term which corresponds to the energy of a single PTCDA molecule in gas phase after relaxation. Hence, at $\Theta = 1.0$, the difference between Eqs. (7) and (8) corresponds approximately to the formation energy of the monolayer. All terms in Eqs. (7) and (8) are calculated at the given coverage value of Θ .

For the calculations with Θ of 0.60, 0.45, 0.30, and 0.15 ML, we have modelled the system with a larger surface unit cell with area of 824 Å² and a slab consisting of three layers each with 110 atoms of Au. The surface unit cell in this model is rectangular with unit cell vectors of magnitude $a = 32.352$ Å and $b = 25.471$ Å. At $\Theta = 0.60$, the coverage corresponds to the adsorption of four molecules in a herringbone arrangement on top of the surface unit cell, thus being consistent with our above-given definition of monolayer coverage ($\Theta = 1.0$). Therefore, coverages of 0.45, 0.30, and 0.15 ML correspond to the adsorption of 3, 2, and 1 molecule(s) on the same surface unit cell. For these calculations, we chose the size of the vacuum gap to be approximately 50 Å and a Monkhorst-Pack⁷ grid of $2 \times 2 \times 1$ k-points in the reciprocal space. We performed the structural relaxation of the system using the PBE+vdW^{surf} method only at $\Theta = 0.60$ ML by fixing the Au atoms in the two bottom

TABLE I. Specifications for the unit cell of each structure investigated for PTCDA on Cu(111).

Structure	Surface Unit Cell	Area [Å ²]
1	$\begin{pmatrix} 6 & 2 \\ -4 & 6 \end{pmatrix}$	252
2	$\begin{pmatrix} 5 & 0 \\ -5 & 10 \end{pmatrix}$	286
3	$\begin{pmatrix} 7 & 2 \\ -4 & 6 \end{pmatrix}$	286

layers. For this structural relaxation, we did not take into account vdW interactions between metal atoms and used *light* settings. The remaining model systems with Θ of 0.45, 0.30, and 0.15 ML were built from the system at $\Theta = 0.60$ ML. Van der Waals interactions were taken into consideration only in the calculation of the final adsorption energies using *tight* settings and Eqs. (7) and (8).

4. PTCDA on Cu(111)

In the case of PTCDA on Cu(111), a larger unit cell in comparison to Ag and Au is required due to the smaller lattice constant of Cu. We used three models, derived by Romaner *et al.*²³, which are based on experimental data²⁴: structure 1, 2, and 3. The three structures have two inequivalent PTCDA molecules per unit cell and were modeled with slabs consisting of three metallic layers. All slabs were generated with the PW91 lattice constant which is 3.638 Å²³. Structure 1 consists of a $\begin{pmatrix} 6 & 2 \\ -4 & 6 \end{pmatrix}$ surface unit cell with 44 metal atoms per layer and a unit cell area of 252 Å², while structure 2 and 3 are created using a $\begin{pmatrix} 5 & 0 \\ -5 & 10 \end{pmatrix}$ and a $\begin{pmatrix} 7 & 2 \\ -4 & 6 \end{pmatrix}$ surface unit cell, respectively. Both cells are conformed with 50 atoms per metallic layer and a unit cell area of 286 Å². We chose the size of the vacuum gap to be approximately 25 Å and a Monkhorst-Pack⁷ grid of $2 \times 2 \times 1$ k-points in the reciprocal space. We performed the structural relaxation of the system using the PBE+vdW^{surf} method by fixing the Cu atoms in the two bottom layers. For the structural relaxations, we did not take into account vdW interactions between metal atoms in order to avoid an artificial relaxation of the surface due to the fact that the surface slab was created using the PW91 lattice constant. They were taken into consideration only in final adsorption energy calculations. All relaxations were performed using *light* settings as described above. Final adsorption energies were calculated with *tight* settings, a Monkhorst-Pack grid of $4 \times 4 \times 1$ k-points in the reciprocal space, and taking into account vdW interactions between metal atoms. The adsorption energies were calculated with Eqs. (7) and (8) with $N = 2$.

F. Nitrogen-containing systems on Metal Surfaces

Adsorption model and calculation settings

Calculations have been performed with the pseudopotential plane-wave code CASTEP-6.0.1²⁵ using Materials Studio library ultrasoft pseudopotentials²⁶.

All calculations were performed with (6×4) and (6×5) frozen (111)-oriented 4-layer surface slabs of Ag and Au with 350 eV or 450 eV plane wave cutoff for Azobenzene (AB) and 3,3',5,5'-tetra-tert-butyl-Azobenzene (TBA), respectively. The lattice constants used for Ag and Au are 4.14 Å and 4.19 Å respectively. The first 2 substrate layers of Ag(111) and Au(111) were relaxed previous to adsorption of AB. For both surfaces, the frozen substrate is believed to be a good approximation due to only minimal structural changes upon adsorption. The vacuum region was chosen to exceed 20 Å. All energy differences and adsorption energies were calculated for these 4-layer metal slabs at a $8 \times 4 \times 1$ Monkhorst-Pack⁷ k-space integration grid for Azobenzene systems and a $6 \times 4 \times 1$ grid for TBA systems. Relative energies and adsorption energies are converged to ± 25 meV with respect to plane-wave cutoff, k-space integration, and vacuum spacing. Additional details on computational parameters that have been set can be found in Ref. 27. Molecular geometries were generated by geometry optimization down to a maximum force component of 25 meV/Å. Calculations of the gas-phase molecules have been performed in $(40 \text{ Å} \times 40 \text{ Å} \times 40 \text{ Å})$ and $(50 \text{ Å} \times 50 \text{ Å} \times 50 \text{ Å})$ rectangular supercells for AB and TBA with the electronic structure calculated only at the Γ -point of the first Brillouin zone.

II. HIOS BENCHMARK DATASET

The mean absolute deviations (MADs) discussed in the main manuscript are calculated via

$$\text{MAD} = \frac{1}{N} \sum_i |x_i - x_{\text{exp}}|, \quad (9)$$

where x_i refers to the observable as given by the electronic structure method, x_{exp} corresponds to the experimental reference value, and N is the number of data-points. For the calculation of MADs we have used experimental reference values of 23 different vertical adsorption heights and 17 adsorption energies that are listed in Table II.

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TABLE II. Experimental reference values of adsorption heights and energies. For references see main manuscript.

system	d in Å	E_{ad} in eV	comment
Xe/Pt(111)	3.40	0.270	Xe–Me distance
Xe/Pd(111)	3.07	0.320	Xe–Me distance
Xe/Cu(111)	3.60	0.187	Xe–Me distance
Xe/Cu(110)	3.30	0.218	Xe–Me distance
Xe/Ag(111)	3.60	0.211	Xe–Me distance
Bz/Cu(111)	–	0.69	average C–Me distance
Bz/Ag(111)	3.04	0.68	average C–Me distance
Bz/Au(111)	–	0.65	average C–Me distance
Bz/Pt(111)	2.02	2.19	average C–Me distance
Np/Cu(111)	–	1.07	average C–Me distance
Np/Ag(111)	–	1.04	average C–Me distance
Np/Pt(111)	–	2.19	average C–Me distance
DIP/Cu(111)	2.51	–	average C–Me distance
DIP/Ag(111)	3.01	–	average C–Me distance
DIP/Au(111)	3.17	–	average C–Me distance
C60/Ag(111)	2.01	–	C– average 1st layer distance
C60/Au(111)	1.80	–	C– average 1st layer distance
Tp/Au(111)	–	0.66	S–Me distance
Tp/Ag(111)	–	0.56	S–Me distance
Tp/Cu(111)	2.62	0.68	S–Me distance
PTCDA/Ag(111)	2.86	–	average C–Me distance
PTCDA/Ag(111)	2.86	–	average O–Me distance
PTCDA/Ag(100)	2.81	–	average C–Me distance
PTCDA/Ag(100)	2.64	–	average O–Me distance
PTCDA/Ag(110)	2.56	–	average C–Me distance
PTCDA/Ag(110)	2.33	–	average O–Me distance
PTCDA/Au(111)	3.34	1.93	average C–Me distance
PTCDA/Cu(111)	2.66	–	average C–Me distance, model 3
PTCDA/Cu(111)	2.81	–	average O–Me distance, model 3
AB/Ag(111) 210 K	2.97	1.02	average N–Me distance