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Chiral Adsorption

N-Heterocyclic Carbene vs. Thiophene – Chiral Adsorption and Unidirectional Rotation on Au(111)

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Abstract: *N*-Heterocyclic carbenes are highly effective ligands for anchoring functional organic molecules to metal surfaces and nanoparticles, facilitating the formation of self-assembled monolayers. However, their adsorption on surface is difficult to predict and control, and there is an ongoing debate on the geometry of NHC derivatives on gold surfaces and on the role of gold adatoms. We present two single molecules based on a benzimidazole NHC, one equipped with a thiophene substituent, and the other ending with a Br atom. By low temperature scanning tunneling microscopy we show that both molecules adsorb planar on Au(111) and are chiral on the surface. Our results indicate that in both cases a complex between NHC and a gold adatom is formed. Upon voltage pulses with the STM tip, both complexes move excited by inelastic tunneling electrons. For the derivative with thiophene, we observe a stepwise 60° unidirectional rotation around the S atom. The direction of rotation is determined by both the chirality and the position of the applied pulse. On the contrary, the NHC derivative without thiophene moves laterally on the surface. Adsorption, binding to gold atoms, and motion are discussed with the support of density functional theory calculations and image simulations.

N-Heterocyclic carbenes (NHCs) have emerged as promising ligands for self-assembled monolayers (SAMs) on metal surfaces and nanoparticles. Due to their ability to form a strong covalent bond to gold and their unique electronic properties, NHCs represent an alternative to thiol-based anchors for surface modification.[1]

The first studies of the adsorption and diffusion properties of single NHC molecules on a gold surface by scanning tunneling microscopy (STM) were carried out to understand how NHC SAMs are formed.[2] These studies revealed an apparent contradiction: although NHCs are known to bind strongly to gold, they often show a high mobility on the Au(111) surface. Based on these results, the adsorption mode of NHCs on gold and the role of the surface (ad)atoms have been the subject of investigation and debate: It was proposed that upon adsorption, NHCs form a single stable covalent bond with a gold atom.[3] However, depending on lateral groups, coverage, and other factors, the gold atom can either belong directly to the surface, resulting in a strong anchoring of the NHC, or it can be an adatom on the surface, forming a highly mobile organometallic complex.[2,4] In the latter case, the motion of the vertically adsorbed NHC–Au complex was defined as a "ballbot type" motion. Additional studies have confirmed the formation of the NHC–Au bond[3] and also the two possibilities of Au atoms bound to the NHC. Another interesting point is the adsorption geometry on the surface, and the conditions required for a vertical or a planar adsorption geometry. The vertical adsorption of NHC-based compounds was initially described, in agreement with the results on SAMs. Further investigations revealed however a quite large spectrum of different adsorption geometries, where the NHC group is not always oriented vertical to the surface, but in several cases also planar and flat. A variety of slightly different studies suggested that the adsorption geometry depends on the specific molecular structure, with the carbene carbon

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always forming a single bond with a gold atom (either inside the surface or as an adatom).[3,5] However, even for rather simple NHCs, conflicting reports exist on whether NHCs adopt an upright or flat-lying configuration on the surface.[1b,5c,6] A recent investigation of NHC monolayers on Au thin films under ambient conditions proposed a dynamic binding mode, where the carbene orientation changes from upright to flat with the adsorption time.[7]

NHC is therefore presently emerging as a model system for a novel anchoring group due to its stability and chemical versatility, limited however by puzzling and not fully controllable adsorption properties on the gold surface.

From the point of view of single-molecule machines[8] and for the development of nanoscale molecular devices able of performing calculations,[8a] generating work,[9] or storing energy,[10] the use of NHC–Au complexes can represent a promising design strategy, allowing both vertical and planar geometries with different possible anchoring strength.

The controlled rotation of a single molecule on a surface induced by inelastic tunneling electrons is a fascinating goal of research since long,[11] and a few examples of unidirectional rotation of both planar and vertical anchored molecules induced by tunneling electrons have been reported.[8b,12] Specifically, an example of an NHC-based single-molecule rotor has been recently presented,[13] while diffusing ballbot-type NHCs have been linked together forming covalent chains,[4] suggesting that further design variations towards more complex tunable nanomachines and vertical rotors are possible.

In this work, we investigate the adsorption and motion of NHCs on Au(111) using a benzimidazole NHC with a lateral thiophene substituent (NHC^{i}Pr-T), i. e. a system with two potential binding sites, carbene and sulfur (Figure 1a). A similar molecule carrying a bromo (NHC^{i}Pr–Br) substituent is considered for comparison (Figure 1b).

By low temperature STM supported by DFT calculations we find that upon adsorption on the Au(111) surface both derivatives form NHC–Au complexes with a gold surface adatom each. The metalorganic complexes adsorb flat on Au(111) due to van der Waals interaction. When excited by inelastic tunneling electrons, the thiophene derivative NHC^{i}Pr–T shows a stepwise 60° unidirectional rotation around the S atom, while NHC^{i}Pr–Br is laterally moved on the surface.

The molecular design of the investigated molecules benefits from the facile structural modifications of NHC (see Supporting Information for the synthesis and chemical characterization). In 1,3-diisopropyl-6-(thiophen-2-yl)-1*H*-benzo[d]imidazol-3-ium-2-carboxylate (NHC^{i}Pr–T), the thiophene provides an additional, albeit weak option to anchor, while for 5-bromo-1,3-diisopropyl-1*H*-benzo-[d]imidazol-3-ium-2-carboxylate (NHC^{i}Pr–Br), the thiophene is substituted by a Br atom. In both compounds, the carbene is masked by a carboxylate, which cleaves CO_2 upon heating in vacuum (see also Supporting Information Figure S12).

With the pure NHC carboxylate precursors in hand, sublimation of both NHCs on the Au(111) surface kept at room temperature under ultra-high vacuum (UHV) conditions was carried out (see Supporting Information for details). STM images (Figure 2a,b and Figure S14) recorded at $T = 5$ K show isolated single NHC^{i}Pr–T and NHC^{i}Pr–Br molecules. The molecules adsorb on both FCC and HCP terraces (see overviews with surface reconstruction in Figure S14, also indicating the surface orientation). Different from the previous reports on NHCs standing vertically on the Au(111) surface,[1b,3a,5c,6] both NHC^{i}Pr-T and NHC^{i}Pr–Br adsorb flat on Au(111) in all observed cases.

In the STM images, NHC^{i}Pr–Br (Figure 2b, Figure S14b) appears very similar to NHC^{i}Pr–T (Figure 2a, Figure S14a) but shorter due to the absence of the thiophene group (see Supporting Information Figure S15 for a direct comparison). Furthermore, NHC^{i}Pr–Br is very mobile on the surface also at low temperature, and its imaging is possible only for very low tunneling current ($I < 10$ pA). In some cases, it forms dimers where two molecules interact at the Br position (Figure S14).

Both molecules are pro-chiral, i. e. two different conformations with mirror symmetry result when adsorbed on a

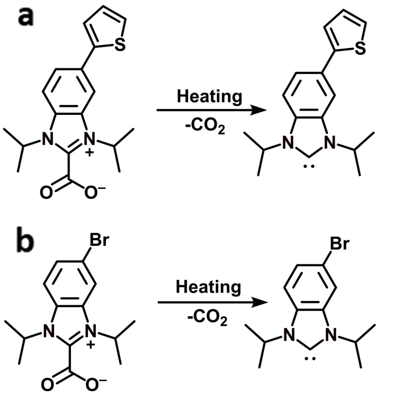

Figure 1. (a) NHC^{i}Pr–T and (b) NHC^{i}Pr–Br carboxylate precursors before and after heating. CO_2 elimination is thermally induced upon sublimation.

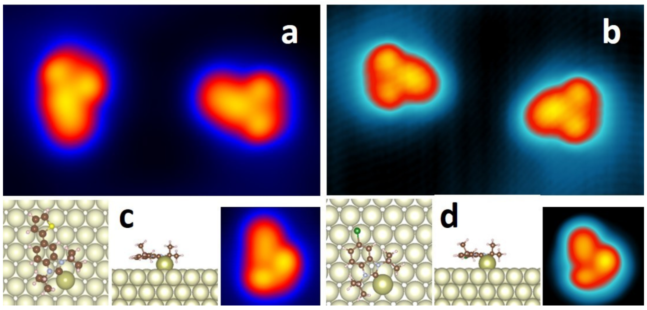

Figure 2. Experimental STM images of (a) NHC^{i}Pr–T and (b) NHC^{i}Pr–Br adsorbed on the Au(111) surface, displaying two chiralities. Images size: 5 nm × 3 nm, $V = 0.2$ V, (a) $I = 50$ pA, (b) $I = 7$ pA due to the high mobility of the molecule. Adsorption geometry of (c) NHC^{i}Pr–T and (d) NHC^{i}Pr-Br on Au(111) with a gold adatom at the carbene carbon atom calculated by DFT and corresponding calculated STM images (image size: 2 nm ×2 nm, $V = 0.5$ V).

surface. Both chiralities appear nearly uniformly present on the surface.

To determine the adsorption geometry of the molecules on Au(111), density functional theory (DFT) calculations and STM image simulations for different possible geometries were performed (See Supporting Information for details). The energetically most favorable cases shown in Figure 2c,d. present planar adsorption geometries with a gold adatom bound at the carbene carbon position. The corresponding calculated STM images are in very good agreement with the experimental ones, confirming for both molecules the formation of a NHC–Au complex with a gold adatom. Calculations of further geometries are reported for comparison in the Supporting Information Figure S22, also confirming the CO_2 cleaving. Interestingly, DFT calculations also show that NHC^{i}Pr–T could eventually stand upright if bound to a gold atom belonging to the surface, and not to an adatom as in the present case (see Supporting Information Figure S22c), suggesting that a full monolayer of molecules might lead to a vertical adsorption. Concerning the origin of the gold adatoms, they can be extracted by the molecule from the gold surface,[2] or be diffusing gold adatoms[14] as reported in several examples of surface metal-coordination bond involving Au adatoms.[15]

In order to study the movement of the molecules on the surface and the role the thiophene group, we induced inelastic tunneling electrons on both NHC^{i}Pr-T–Au and NHC^{i}Pr–Br-Au complexes, as shown in Figure 3. This is done by vertically positioning the tip on a precise position of the molecule and applying a voltage for a defined time, keeping a constant tunneling current. A typical voltage pulse of 0.5 V with a duration of 10 s induces different movements on the two adsorbed molecules.

During a voltage pulse, NHC^{i}Pr-T–Au rotates around the thiophene group in steps of 60° (Figure 3a-c), while a lateral movement is prevented. On the contrary, NHC^{i}Pr-Br–Au translates on the Au(111) surface (Figure 3d-f). In Figure 3a–c, two steps of rotation of a D enantiomer of NHC^{i}Pr–T-Au are shown. A pulse applied at the position of the white star on the side opposite to the thiophene produces the 60° clockwise movement around the thiophene, schematically indicated by the green arrow, while the position of the molecule after the pulse is shown in Figure 3b. A second pulse (Figure 3b–c) causes a further 60° rotation in the same direction. Similarly, a pulse applied at the same side of the thiophene causes a 60° anti-clockwise rotation, while the opposite chirality shows the opposite behaviors (see Supporting Information Figure S19 and S20). The position of the tip needed to produce the rotation corresponds to the lateral CH on the central ring, either on the right or on the left side. The rotation angle of 60° is related to the adsorption geometry on the hexagonal Au(111) surface.[12d] Negative voltage pulses bring to uncontrolled rotations. Further positions have been tested but do not produce any reliable and controlled rotation.

In Figure 3d-f, two translations of a L enantiomer of NHC^{i}Pr–Br-Au are reported for comparison induced by similar voltage pulses. Notably, the tunneling current is kept in this case much lower, to avoid uncontrollable movements.

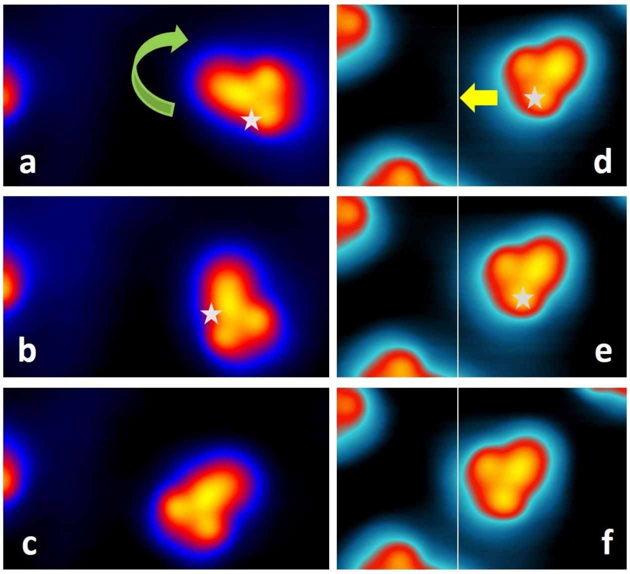

Figure 3. (a) STM image of a single D enantiomer of NHC^{i}Pr-T–Au. By applying a voltage pulse $V=0.6$ V and $I=1$ nA at the position of the white star, the molecule rotates of 60° in the clockwise direction around the thiophene; (b) STM image recorded after the application of the voltage pulse in (a). A further pulse is applied at the position of the white star causing a further 60° anticlockwise rotation; (c) STM image of the molecule after the second voltage pulse. (a–c): Image size 4.5 nm × 2.5 nm, $V=0.2$ V, $I=50$ pA; (d) STM image of a single L enantiomer of NHC^{i}Pr–Br-Au. By applying a voltage pulse $V=0.5$ V and $I=0.05$ nA at the position of the white star, the molecule translates in the direction of the yellow arrow. (e) STM image recorded after the application of the voltage pulse in (d). A further pulse is applied at the position of the white star causing a further lateral movement; (f) STM image of the molecule after the second voltage pulse. (d-f): Image size 3 nm × 2.5 nm, $V=0.2$ V, $I=7$ pA. The white vertical line is a guide to the eye.

Both rotation of NHC-^{i}Pr-T–Au around the sulfur and translation of NHC^{i}Pr–Br-Au indicate that the NHC–Au complexes are mobile on the gold surface. This result is in agreement with the previously observed motion of the vertical ballbot,[2,4] which is a similar complex of NHC and a gold adatom. In the present case, however, the planar adsorption and the presence of the thiophene limits the diffusion and favors the rotation.

A complete 360° step by step anticlockwise rotation of a L NHC^{i}Pr-T–Au is shown in Figure 4a. By superposing the STM images before and after the rotation, we determined the axis of rotation, indicated by the cross in Figure 4a (se Figure S16). A more precise experiment reported in the Supporting Information indicates that the anchoring point corresponds to the position of the sulfur atom (Figure S17). DFT calculations confirm that for NHC-^{i}Pr-T–Au, the energy barrier for translation is higher than the energy barrier for rotation around the sulfur atom (see Figure S23).

The NHC^{i}Pr–T molecules have a length of about 1.4 nm, while most of the FCC and HCP terraces of Au(111) measure less than 3 nm (see overview in Figure S14a), making it unlikely that the complete rotation of the

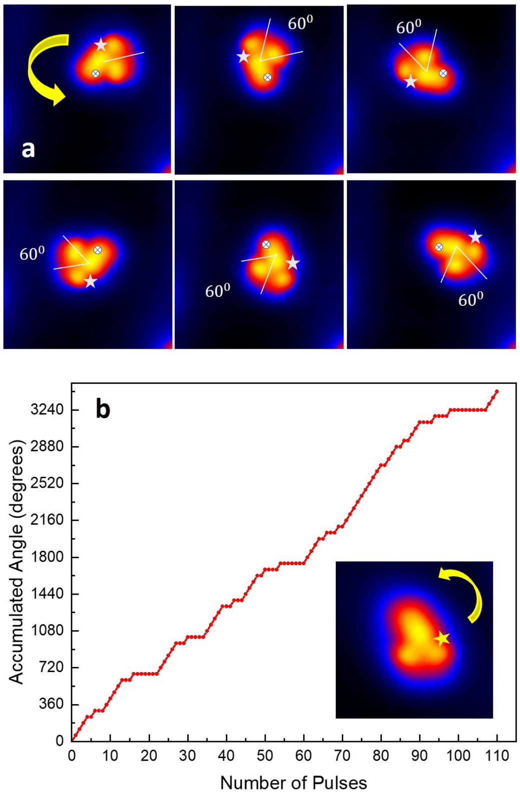

Figure 4. (a) STM images (size: 5 nm x 5 nm, I = 20 pA, V = 0.2 V) of a pre- and post-pulsed (pulse parameter: V = 1 V, I = 1 nA) L NHC^{i}Pr-T–Au complex exhibiting a complete anticlockwise rotation in steps of 60°, where the pulse position is marked with a white star and the anchoring point is marked with a cross. The yellow arrow indicates the direction of rotation. (b) Successive accumulated rotation angles for 111 consecutive voltage pulses on a L molecule. Positive angles indicate anticlockwise direction. The inset show the STM image of the molecule. The star indicates the position of the pulse, and the yellow arrow the direction of rotation. STM image size: 2.75 nm × 2.75 nm, at 20 pA, 0.2 V. Pulsing parameters: V = 0.4 V–1.3 V, I = 0.5 nA–1 nA.

NHC–Au complex takes place without interacting with the soliton lines. This interaction hampers the rotation, so that a higher voltage or tunneling current is needed to pass over the soliton lines. When the molecule is adsorbed in the center of a terrace and far enough from others, the rotation can be reproduced without changing parameters for several complete rounds, as depicted in the example of Figure 4a.

In Figure 4b, we have plotted the successive accumulated rotation angles observed in 111 consecutive applied voltage pulses on a typical single L molecule (shown in the inset) by pulsing on the right side (anticlockwise rotation) as indicated by the yellow star. We observe a monotonic increase of the successive accumulated rotation angle without any back rotation. In some cases, the molecule does not further rotate (typically when it is too close to a reconstruction line, as discussed earlier) and the voltage and current of the pulse must be increased after a few unsuccessful attempts to pass the reconstruction line. This is shown by the plateaus in the monotonic lines of Figure 4b, which appear relatively regularly after every 6th pulse, indicating that the complex tends to block at the same position every turn.

An example of the rate for rotation versus the applied voltage at a tunneling current I = 1 nA is presented in the Supporting Information Figure S21. We observe a yield of about $1\text{x}10^{-12}$ rotations/electron at a bias voltage V ~400 mV, which increases to $1\text{x}10^{-10}$ rotations/electron at V ~800 mV. This behavior is compatible with the inelastic tunneling excitation of a C–H stretch vibrational mode (at 370 meV),[8b] but also of excited electronic states.[16] A direct effect of the tip-molecule interaction is negligible, since the manipulation is performed at a tunneling resistance of about 1 G Ohm. i. e. with the tip vertically far from the molecule.

In general, unidirectional rotation of an adsorbed molecule is possible without violating the microscopic reversibility principle if electronic excited states are involved in the process.[8b,c] In a STM voltage pulse experiment this condition is fulfilled because excited molecular electronic states can be partially occupied during the electron tunneling through the molecule. A second necessary ingredient for unidirectionality is an asymmetry or conical intersection between the excited and ground electronic potential energy surfaces. A key structural factor enabling this asymmetry is chirality.[17] In the present experiment both chirality and electron tunneling are present, qualitatively explaining the observed unidirectional rotation.

In conclusion, we presented the study of *N*-heterocyclic carbenes (NHCs) with two different substitutions on the Au(111) surface. STM images show that both types of molecules adsorb flat and are chiral upon adsorption on the surface. They form a complex with a gold adatom via the carbene, as confirmed by DFT simulations. The NHC complex carrying a thiophene (NHC^{i}Pr-T-Au) is anchored on Au(111) via the sulfur atom, thus allowing unidirectional rotation by voltage pulses with the STM tip. The direction of rotation is determined by the position of the tip and the chirality of the molecule. The complex without thiophene (NHC^{i}Pr–Br-Au) easily diffuses on the surface and shows lateral displacement by voltage pulses. Compared to previous experiments on NHCs on Au(111), we do not observe molecules standing upright. This study contributes to the ongoing debate on the adsorption geometry of NHC derivatives on gold surfaces and on the role of gold adatoms. Towards the design of NHC-based vertical molecules motors and switches, it is still necessary to fully understand in which conditions NHCs are standing upwards and which functional groups can be connected to NHC without affecting the verticality on the Au(111) surface.

Supporting Information

A Supporting Information PDF file is available containing the synthesis and chemical characterization of the two molecules, and supplementary experimental results and calculations.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords: NHCs · Carbides · Molecule-rotor · Scanning probe microscopy · Chirality

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Communication

Chiral Adsorption

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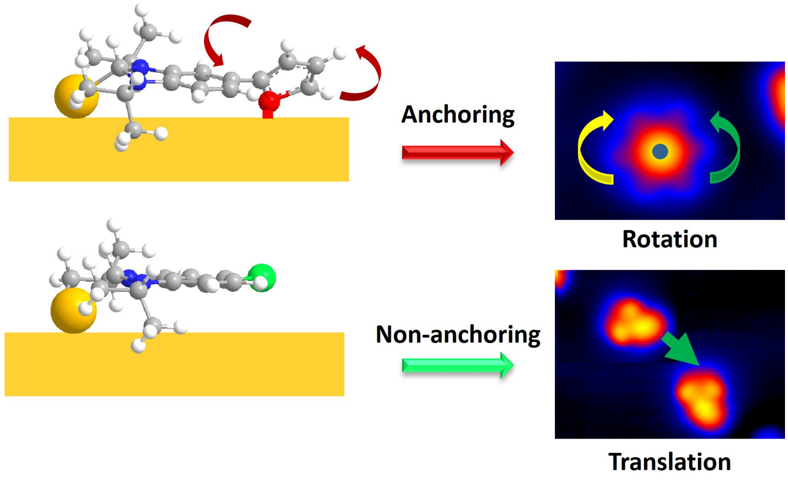
N-Heterocyclic Carbene vs. Thiophene – Chiral Adsorption and Unidirectional Rotation on Au(111)



Single NHC molecules carrying a thiophene (NHC^{i}Pr–T) and a bromo (NHC^{i}Pr–Br) substituent are investigated by STM on the Au(111) surface. Both derivatives adsorb flat on the surface and are bound to a gold adatom via the carbene. NHC^{i}Pr–T is anchored to Au(111) via the sulfur atom, thus allowing unidirectional rotation by voltage pulses with the STM tip. In comparison, NHC^{i}Pr–Br shows lateral displacement by voltage pulses.