Surface Science 709 (2021) 121837

Contents lists available at ScienceDirect

Surface Science

journal homepage: www.elsevier.com/locate/susc

Conformational behavior of naphtho-merocyanine dimers on Au(111)

Andreas Riemann [*], Lucas Browning, Hunter Goff

Department of Physics and Astronomy Western Washington University, Bellingham, WA 98225, United States

ARTICLE INFO

Keywords:
Merocyanine
Spiropyran
Molecular mechanics
DFT
STM
Dimer formation

ABSTRACT

Thin film growth of molecules on substrates are governed by the convolution of inter-molecular forces and template-adsorbate interactions. Often the initial dimer formation plays a crucial role in the outcome of the molecular structure on the surface. Here, the behavior of naphtho-merocyanine on an Au(111) substrate was investigated using computational chemistry methods and Scanning Tunneling Microscopy. The experiments show a strong preference of dimer formation of the merocyanine molecules. Topographical measurements are used to identify two distinguished configurations, an elongated/oval dimer and a compact/rectangular dimer. With the addition of computational chemistry calculations including Density Functional Theory (DFT) and Molecular Mechanics calculations using the AMBER 3 force field, these two configurations of two specific merocyanine conformers, namely CTC and CTT, could be identified. Intermolecular binding energy calculations could be performed. This is a first step in understanding the possible island/thin film growth of naphtho-merocyanine and subsequently possible pathways toward the switching behavior of merocyanine and spiropyran on this substrate.

1. Introduction

Molecular switches on substrates are an important sub-class for functionality of molecular electronics. Two or more isomers with different conductance can be used as an electronic switch in molecule-based devices [1–6]. The switching properties and thresholds are influenced by the interaction of these molecules with the underlying substrates [7–9]. For instance, metallic substrates can introduce additional excitation routes of molecular switching due to their reservoirs of electrons and holes [10,11]. However, other studies have shown that adsorption on metallic substrates could also lead to a loss of photo-isomerization [12–14]. Using different types of substrates, the electronic properties of semi-conductors and other non-metals can suppress switching mechanisms due to electronic surface features which means the switching process can be better controlled by external stimuli [15]. Overall, the combination of a suitable substrate and a molecular switch with appropriate end groups can lead to a sufficiently high photo-isomerization potential [16]. As a stimulus, light for instance has various advantages: it can be used to stimulate the switch locally with high precision, it can be tuned to specific wavelengths and energies, and it does not introduce any contamination to the molecular structure. Switches activated by heat usually are stimulated over a wider area of the sample. Studies have shown that environmental factors, such as Ultra-High Vacuum vs. ambient conditions, can also create differences in the isomerization processes and yield [17].

A promising candidate chosen for the present study of molecular switches is a naphtho-spiropyran/merocyanine molecule (see Fig. 1). In general, the class of spiropyran/merocyanine molecules is especially interesting for a variety of applications since their isomers have very different properties. Spiropyran (SP) molecules consist of an indoline and a benzopyran unit connected together via a spiro junction. Cleavage of the central C–O bond leads to the creation of a merocyanine (MC). This class of molecules can undergo reversible isomerization caused by a variety of stimuli depending on the environment of the molecule. The switching between these isomers has been investigated extensively in solution, and only recently on selected metal substrates [11,18–20]. The class of SP/MC-based molecules is especially interesting since the isomers have vastly different properties concerning the size, dipole moment, color, and emission properties. Both isomers are structurally very distinguishable: spiropyran is a three-dimensional molecule where the spiro junction leads to aromatic rings being at 90° angles. However, the merocyanine with the central C–O bond broken is a much more planar molecule. These properties play an important role in their adsorption behavior when anchored to a substrate. The charge separation within the molecule leads to pronounced dipole moments in both, the spiropyran and the merocyanine isomers. Density Functional Theory

---

* Corresponding author.
E-mail address: andreas.riemann@wwu.edu (A. Riemann).

https://doi.org/10.1016/j.susc.2021.121837
Received 11 December 2020; Received in revised form 22 February 2021; Accepted 24 February 2021

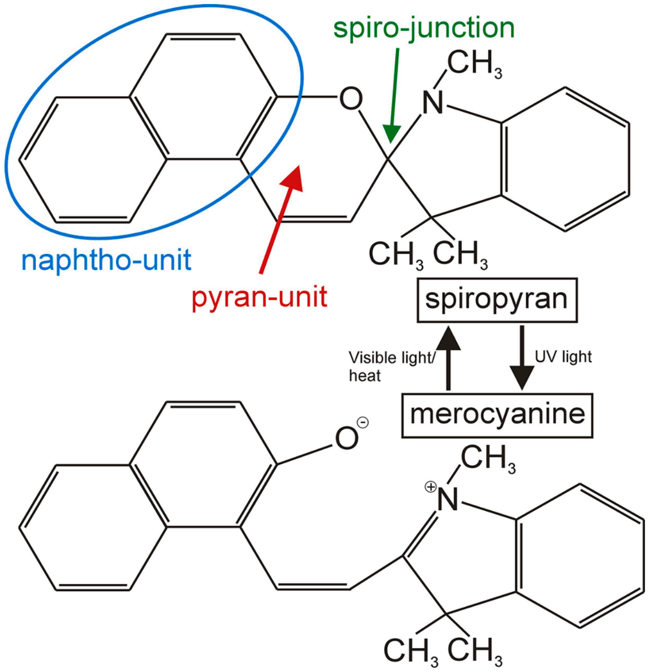

Fig. 1. Conformation of naphtho-spiropyran (top) and naphtho-merocyanine (bottom), indicated are the naphtho-unit (left end), the central pyran unit, and the spiro junction. Cleaving of the central C–O bond transforms the spiropyran isomer into the merocyanine isomer through UV light illumination in solution. The reverse reaction from merocyanine to spiropyran by reestablishment the central C–O bond can be facilitated in solution through illumination with visible light or heat.

(DFT) calculations as well as electro-optical absorption measurements have shown that the dipole moment of the merocyanine molecules is much bigger than that of spiropyran, increasing from about $(10-15)\times 10^{-30}$ C·m to $(50-60)\times 10^{-30}$ C·m, or by a factor of 4 to 5 [21,22]. The optical properties of spiropyran-based molecules in solutions are well known for over half a century [23,24]. The spiropyran isomer is colorless, meaning optically transparent in the visible region. However, the merocyanine isomer absorbs strongly in the yellow region of the spectrum (550 nm–600 nm) and therefore appears blue. Additionally to these absorption behavior differences, the isomers also differ in their emission properties. Spiropyran does not show a strong emission, however, merocyanine has a strong red emission region around 650 nm. The photochromic behavior of this class of molecules is very interesting for a wide variety of applications such as reusable sensors, high-resolution imaging in biological samples, and detection and imaging of mechanical stress [25].

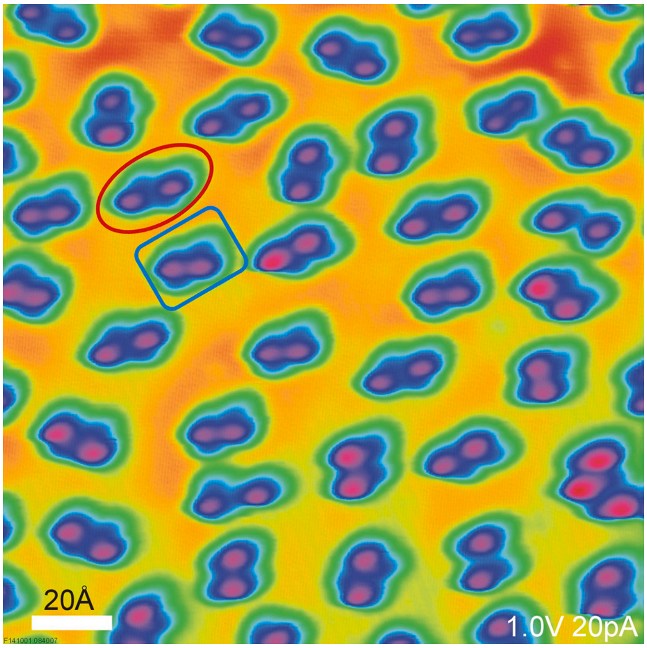

Fig. 2. STM image of merocyanine dimers on Au(111). Image size: 200 Å × 200 Å, parameters: $V = 1.0$ V, $I = 20$ pA. Indicated are two distinguished shapes of dimers: elongated/oval dimers (red) and more compact/rectangular dimers (blue). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In order to achieve large scale molecular domains which can be used as molecular switch, film growth of these molecules has to be established. Many factors play crucial roles during the adsorption interactions, one of them the initial dimer formation between two molecules [26]. Energetically favorable configurations of dimers in anti-parallel orientation (a rotation of $^{180^{\circ}}$ around the axis along the surface normal) can lead to repulsive interactions between dimers and therefore to self-organized growth of molecular wires [27]. On the other hand, dimers oriented in chevron orientation can be the building blocks of wide-scale island/film growth [28]. In all events, the configuration of the initial dimers can be used as a precursor to larger scale adsorption studies necessary for molecular switches.

The present study investigates naphtho-spiropyran/merocyanine adsorption on Au(111) for the first time. Previous studies have looked at other, related molecular switches on gold or on semimetals [13,29,30], however, the specific adsorbate/substrate combination used here has not been investigated. The aforementioned studies have researched various reaction paths for the switching between the spiropyran/merocyanine isomers, the present case investigates the behavior of annealing/heat. Lastly, the combination of microscopic imagining combined with computational chemistry allows for the first time to explore geometries, identify isomers of merocyanine, and calculate adsorption and binding energies for the Naphtho-SP/MC on Au(111) system.

2. Experiment and methods

2.1. Experiment

The molecule for this study was a commercially purchased naphtho-spiropyran molecule (TCI: 1,3,3-Trimethylspiro[indoline-2, $3^{'}$-[3H] naphth[2,1-b]pyran] – $C_{23}H_{21}NO$) at $\geq$98.0% purity. A Lewis structure of this naphtho-spiropyran and naphtho-merocyanine molecule can be seen in Fig. 1.

All experiments were carried out under UHV conditions at pressure of about 5×10^{-10} mbar. The Au(111) sample was cleaned through repeated Ne^{+} sputtering cycles and subsequent annealing of the sample to 750 K. Afterwards naphtho-spiropyran molecules were evaporated at a temperature of 373 K onto a sample held at 245 K. The sample was then cooled down to about 5 K for imaging in the STM. However, only unordered structures consisting of weekly bonded spiropyran clusters were observed under these conditions. These clusters had apparent heights of about 3.2 Å and lateral sizes of about 40 Å. These three-dimensional structures are believed to be clusters of unordered naphtho-spiropyran molecules. The three-dimensional appearance of SP (in contrast to the more planar structure of MC) and possible much weaker adsorption properties are supporting these findings, and no further investigations were carried out on these clusters. In a subsequent preparation step the sample was heated up to 288 K before again being cooled down to 5 K for imaging.

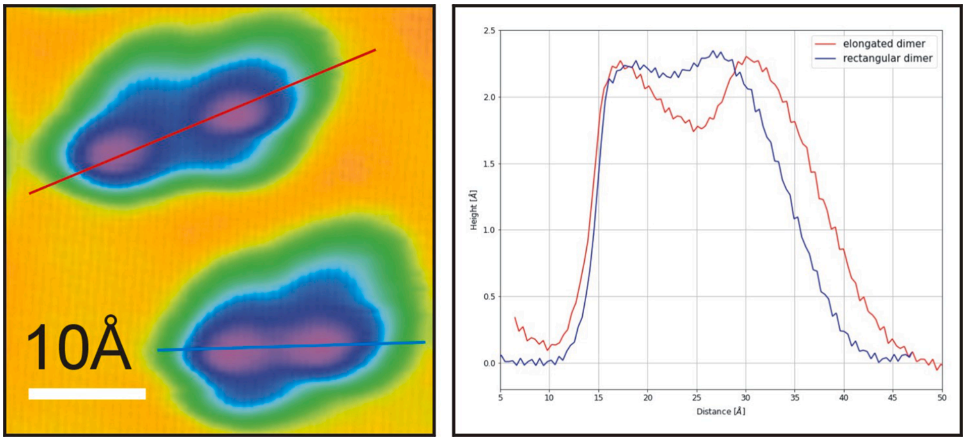

Fig. 3. STM image (enlarged) of both dimer types: elongated (top) and rectangular (bottom) including apparent height profiles (right). Both dimers appear with the same height but the separation of highest points are different by about 3 Å.

2.2. Calculations

The DFT calculations were carried out using ORCA [31]. The molecules were geometry optimized with DFT B3LYP/G employing the 6-31G* basis set. Additionally, energy levels for the molecules, specifically the LUMO levels, were calculated and compared with STM data. Using the DFT B3LYP/G approach partial atomic charges for each isomer/conformer were calculated using Mulliken population analysis [32, 33]. The substrate was modelled as a periodic structure consistent with the Au(111) surface geometry.

After optimizing all molecules with DFT, adsorption energies, adsorption geometries as well as binding energies were calculated using HyperChem and Molecular Mechanics with the force field AMBER 3. Molecular Mechanics in general, and the AMBER 3 force field in particular, have been shown to yield accurate results for adsorption studies of different molecules on Au(111). This approach was used, e.g., to compare experimental and computational data for the adsorption of DNA bases on Au(111) [34], adsorption of amino acids on Au(111) [35], as well as the self-assembly of a chiral molecular honeycomb structures on Au(111) [36]. In these studies, conformational agreement between experimental and computational results could be shown. Adsorption energies on substrates and binding energies between molecules are often less reliable in their absolute values, however, these studies have shown agreements of the relative strength of the interaction between molecules and substrates. With that in mind, the use of MM with AMBER 3 for the present system of merocyanine/spiropyran molecules adsorbed on Au (111) is an appropriate approach.

3. Results and discussion

Fig. 2 shows a typical STM image of the surface structure taken at a bias voltage of $V = +1.0$ V and tunneling current of $I = 20$ pA. The size of the image is 200 Å × 200 Å. After annealing the sample to a temperature of 288 K, the molecules organize themselves into structures with two pronounced protrusions. The apparent lateral size of these features (> 20 Å) clearly indicates that they can not be a single molecule where two of the aromatic rings would be cause for the protrusions, but that they are two molecules, a dimer. Furthermore, the existences of these dimers indicates attractive interactions between two molecules but repulsive interactions between dimers. This suggests that these two molecules are aligned in an anti-parallel fashion which will be more closely examined using molecular mechanics calculations described below.

Images taken with a positive bias voltage indicate tunneling into the LUMO orbitals of the molecules. The shape and location of these orbitals is analyzed using DFT calculations.

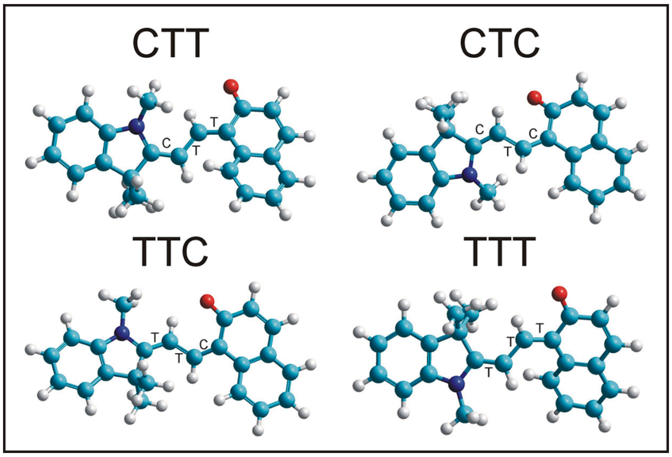

Fig. 4. Stable conformers of naphtho-merocyanine isomer. Labeling of the three central bond orientations of the carbon atoms starts with respect to the nitrogen atom (blue) and end at the carbon next to the oxygen atom (red). All conformers have the middle carbon bond in trans orientation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Most of the dimers can be organized into two categories: elongated/oval-shaped dimers (EO-type) and more compact/rectangular-shaped dimers (CR-type). A closer look at two examples of these molecules can be seen in Fig. 3. Besides their geometric appearance, apparent height profiles have also been taken. Both dimers have a maximum apparent height of about 2.3 Å which indicates the same kind of isomer for both dimers. It is a notably lower height for these species than the one determined for the unstructured original clusters which were attributed to the three-dimensional spiropyran isomers.

3.1. Calculations

The naphtho-spiropyran and naphtho-merocyanine molecules were geometry optimized using the ORCA electronic structure program. Choosing the DFT/B3LYP approach with the 6-31G* basis sets allows the comparison of our data with previous computational chemistry data [37, 38]. The merocyanine isomers can (in general) occur in 8 different conformers distinguished by cis/trans properties of the central three carbon bonds. In our case, we have labeled cis/trans triplets of the isomers starting on the carbon bond closest to the nitrogen atom and ending at the carbon bond closest to the oxygen atom. Due to the geometry of this specific spiropyran/merocyanine molecule with the two

Table 1
Adsorption energies of spiropyran isomer and merocyanine conformers calculated using the AMBER 3 force field. These energies are determined by the difference of the energies of the system when the molecule is adsorbed in its optimal configuration and when the molecule is far away from the substrate, and not interacting with it.

Isomer/conformer	SP	CTT	CTC	TTC	TTT
Energy [eV]	0.34	0.42	0.45	0.47	0.43

Table 2
Binding energies of merocyanine dimers consisting of the four conformers. The energy of the system consisting of the substrate and two adsorbed merocyanine molecules was determined for two different situations. First, the two molecules adsorb at optimized and equivalent lattice locations on the substrate without interacting with each other. The second situation is where two molecules are positioned on the substrate in such a way that their energy is minimized (i.e. red area in Fig. 5). The binding energy of a dimer is determined as the difference in energy of these two scenarios.

Conformer	CTT	CTC	TTC	TTT
Energy [eV]	0.32	0.15	0.25	0.22

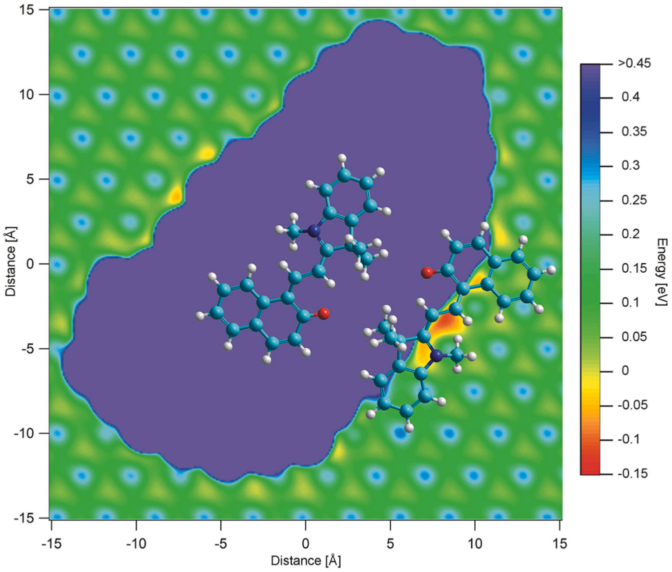

Fig. 5. Energy map, calculated using AMBER 3 force field, for two anti-parallel naphtho-merocyanine molecules, as CTC conformers. The first molecule is fixed at the origin, the second molecule is moved on a lateral grid, and energy of system is calculated. Purple region indicates unfavorable placement of second molecule with very high energy (at places many orders of magnitude higher than 0.45 eV), red region indicates lowest energy (0.15 eV less then the energy for non-interacting molecules). Visible is the periodic underlying substrate structure where adsorption energies follow the surface periodicity. Color scale is in [eV] with energy at zero for non-interacting CTC conformers. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

methyl groups at the indole unit, only isomers with trans configuration for the center carbon bond are stable. The four stable conformers can be seen in Fig. 4. These conformers all show the properties of merocyanine isomers in general of (nearly) parallel aromatic rings. That is in stark contrast to the naphtho-spiropyran molecule where the spiro junction causes a nearly perpendicular arrangement between the indole and pyran rings are at an angle of about $^{90^\circ}$.

The adsorption of spiropyran and the merocyanine conformers on the substrate was calculated using HyperChem with the AMBER 3 force field. The substrate was modeled as a periodic structure with the geometric properties of the Au(111) surface. The first step is to calculate the total energy for the system consisting of the substrate and the molecule, where the molecule is positioned high above the substrate (200 Å away) and, therefore, is not interacting with the substrate. The actual adsorption is calculated by bringing the molecule in close vicinity to the substrate (5 Å above the substrate) and then calculating its optimal configuration. The difference of the energy of this situation and the non-interacting situation is the adsorption energy for the molecule calculated with the AMBER 3 force field.

All 4 merocyanine conformers adsorb in nearly parallel orientation of their aromatic rings with respect to the substrate, whereas spyropyran adsorbs in such a way that the naphtho unit is nearly parallel to the surface but the aromatic rings with the indoline unit are perpendicular to the substrate. This leads to an adsorption energy of about 0.3 eV for SP, however, the MC conformers have an about 30% higher energy (see Table 1).

After the adsorption of a single molecule in its optimal position (defined as the origin), a second identical molecule was added to the substrate, either in parallel or in anti-parallel orientation. Anti-parallel means that the molecule is rotated by 180° with respect to an axis parallel to the surface normal. This secondary molecule was laterally moved around the first, stationary, molecule on a 30 Å × 30 Å grid with 0.1 Å step size. At each point, the total energy of the system was recorded. The result was an energy map as can be seen in Fig. 5. The background of the map indicates the various energy values (from red = lowest to purple = highest) and overlayed are the two molecules used in this approach. Three distinct features can be observed: (i) the periodic nature of the underlying substrate is visible around the edges indicating identical energy values when the secondary molecule is a certain distance away from the stationary (central) molecule, (ii) the middle region (purple) shows very high energies (at places many orders of magnitude higher than the top of the color scale of 0.45 eV), meaning very unfavorable positions for the second molecule, that is an area where the two molecules partially even overlap, (iii) the small red area is the location where the energy is lowest, meaning the secondary molecule's preferred position. The center of mass of this second molecule is positioned at that grid spot. The colorscale is chosen (shifted) in such a way that a binding energy of zero eV would correspond to two adsorbed molecules in identical lattice spots but far enough away from each other so they do not interact (periodic yellow regions closer to the edges). With that choice, the optimal position for a secondary molecule (lowest energy = red region) has a binding energy of 0.15 eV. That means the energy of the system with two molecules, one at the origin and one at the position indicated by the red region, is 0.15 eV lower than the energy of the system with the same two molecules, one again at the origin but the second one at an identical lattice point farther away where both molecule do not interact. Non-optimal positions of the molecule on the lattice are indicated by the light-blue periodic structure (about 0.25–0.3 eV higher than optimal). The purple region in the middle contains energies above 0.45 eV, as a matter of fact, when the secondary molecule is brought in closer proximity than the optimal position, the energy of the system is increasing very quickly to many orders of magnitude higher than the top of the color scale would indicate.

Using these energies calculated with the AMBER 3 force field, binding energies between two merocyanine conformers can be determined from the energies of two molecules at the optimal position (red area in Fig. 5 and corresponding energy maps for all conformer pairs) and two non-interacting molecules. The binding energies for all conformer pairs in parallel orientations were higher than for the configurations in anti-parallel orientation. This fact together with the findings of previous studies of dimer formation on other molecules and the exclusive observation of dimers in the STM images leads to the conclusion that the merocyanine dimers are in fact two conformers in anti-parallel configuration [27,39]. The energy values for these configurations are summarized in Table 2 and the energetically most favorable dimer orientations are depicted in Fig. 6. As can be seen, the CTT

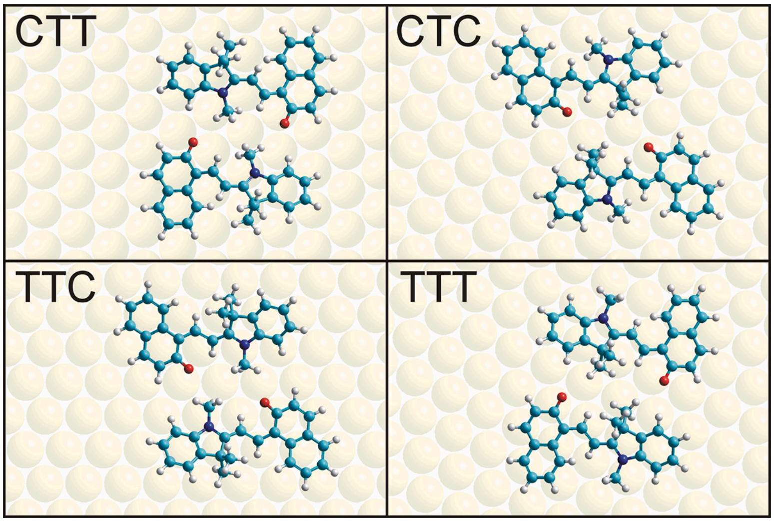

Fig. 6. Anti-parallel configurations of the four dimer conformers, determined by the lowest energy position of two molecules (as seen in an example for CTC in Fig. 5). Notably, the CTT conformers appears the most compact and the CTC conformer most separated.

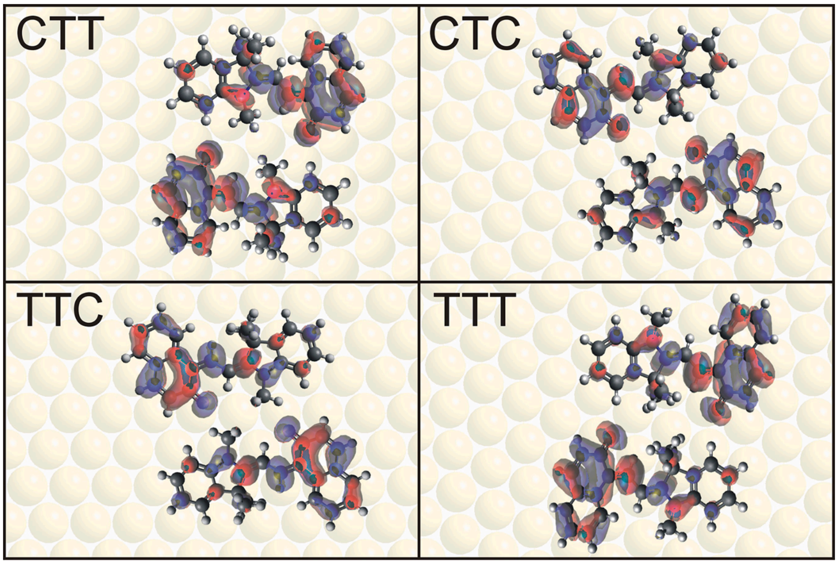

Fig. 7. DFT energy level calculations are used to identify LUMO orbitals for the different dimer conformers. These LUMO orbitals are mostly concentrated at the Naphtho units, e.g. for CTT in the upper right/lower left part.

conformers have the highest binding energy and appear geometrically as the most compact dimer with the oxygen atoms (the red atom in Fig. 6) closest together. The lowest binding energy was calculated for the CTC dimer which geometrically appears the most separated of all four dimers.

As mentioned previously, the STM images of the merocyanine dimers were obtained with a positive bias voltage indicative of tunneling into/imaging the LUMO orbitals of the molecules. Using DFT we performed energy level calculations of all conformers and obtained the LUMO orbital locations as seen in Fig. 7. It is apparent that these orbitals are mostly concentrated around the naphtho units of each merocyanine molecule (e.g. top right and bottom left for the CTT dimers). The locations of the LUMO orbitals can now be matched with the highest contrast of the STM images, and the specific dimers with electronic and geometric concurrence is identified as shown in Fig. 8. Comparing these dimers with their binding energy, it turn out that the STM image appears to show the dimers with the lowest and highest binding energies in these semi-stable configurations. One explanation could be a stronger binding of the molecular end of the naphtho unit with the substrate (since that part of the molecule is “flatter” than the other aromatic rings with additional methyl groups), “fixing” that end to the substrate and only allowing rotation of the one central bond (from CTT to CTC only the carbon bond closest to the naphtho unit would need to rotate).

4. Conclusion

The adsorption behavior of individual naphtho-merocyanine molecules on an Au(111) substrate was investigated using Scanning Tunneling Microscopy (STM) and computational chemistry methods. The experiments show a strong preference of dimer formation of the merocyanine molecule. It should be noted that for the system of naphtho-SP/MC on Au(111), the reaction path between the isomers is different than in solution as in the current system heat drives the reaction towards MC isomers, whereas in solution heat in general drives the reaction toward SP. Topographical measurements are used to identify two distinguished configurations, an elongated/oval dimer and a compact/rectangular dimer. With the assistance of DFT and Molecular Mechanics calculations using the AMBER 3 force field, these two

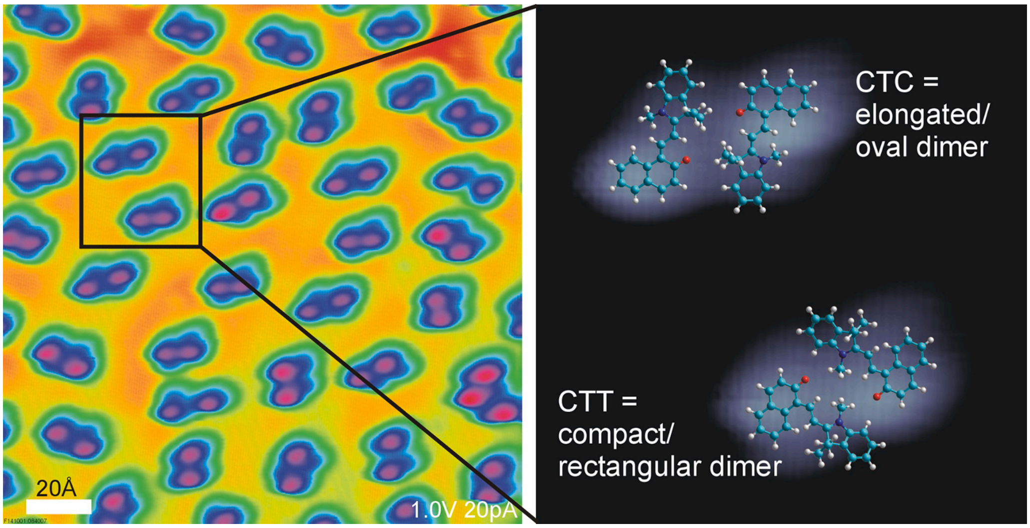

Fig. 8. Matching the STM image with calculated configuration in order to identify the observed dimer configurations. The elongated/oval dimer has been identified as a merocyanine dimer as CTC conformer, and the compact/rectangular dimers as a CTT conformer.

configurations as well as the specific merocyanine conformers, namely CTT and CTC, could be identified and energy calculations could be performed. As found in previous studies on dimers, the constituents of such dimers are two molecules in anti-parallel configuration. This system of molecular adsorption on a metal substrate combined with appropriate computational chemistry methods opens up the opportunity to better understand the underlying processes of island growth of these kind of molecular species. Inter-molecular adsorption geometry are in general a challenge to identify with Scanning Probe Microscopy, however, in combination with Molecular Mechanics and Density Functional Theory further insight can be provided. These findings are a precursor to subsequent island/thin film growth of MC in order to achieve suitable templates for manipulating these naphtho-spiropyran/merocyanine molecular switches. Additionally, in future investigations the functionality of the molecular switch should be tested. As mentioned in the introduction, in solution the reaction of the spiropyran/merocyanine isomers via heat is driven towards spiropyran, however, as shown in the present case annealing created merocyanine dimers. Other stimuli promoting isomeric switching of merocyanine/spiropyran in solution include light at various frequencies; therefore, an expansion of the current study would naturally be the investigation of the switching behavior of merocyanine dimers using visible or UV light.

CRediT authorship contribution statement

Andreas Riemann: Conceptualization, Writing - original draft, Investigation, Visualization, Funding acquisition. **Lucas Browning:** Investigation. **Hunter Goff:** Investigation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work was supported financially by NSF (Grant 1807460). A.R. likes to thank Prof. Katharina Franke for technical support and acknowledge the use of the facilities in her research group at the Freie Universität Berlin.

References

[1] B.K. Pathem, S. Claridge, Y.B. Zheng, P.S. Weiss, Annu. Rev. Phys. Chem. 64 (2013) 605.
[2] A. Plaquet, M. Guillaume, B. Champagne, F. Castet, L. Ducasse, J.-L. Pozzo, V. Rodriguez, Phys. Chem. Chem. Phys. 10 (2008) 6201.
[3] C. Nacci, K. Kanisawa, S. Fölsch, J. Phys.: Condens. Matter 24 (2012) 394004.
[4] F. Kalkan, M. Mehlhorn, K. Morgenstern, J. Phys.: Condens. Matter 24 (2012) 394010.
[5] J. Mielke, S. Selvanathan, M. Peters, J. Schwarz, S. Hecht, L. Grill, J. Phys.: Condens. Matter 24 (2012) 394013.
[6] I.S. Park, Y.-S. Jung, K.-J. Lee, J.M. Kim, Chem. Commun. 46 (2010) 2856.
[7] G. Balasubramanian, J. Schulte, F. Müller-Plathe, M.C. Böhm, Chem. Phys. Lett. 554 (2012) 60.
[8] E. Malic, A. Setaro, P. Bluemmel, C.F. Sanz-Navarro, P. Ordejón, S. Reich, A. Knorr, J. Phys.: Condens. Matter 24 (2012) 394006.
[9] Z. Li, S. Wan, W. Shi, M. Wei, M. Yin, W. Yang, D.G. Evans, X. Duan, J. Phys. Chem. C 119 (2015) 7428.
[10] O. Ivashenko, J.T. van Herpt, B.L. Feringa, P. Rudolf, W.R. Browne, Langmuir 29 (2013) 4290.
[11] M. Piantek, G. Schulze, M. Koch, K.J. Franke, F. Leyssner, A. Krüger, C. Navío, J. Miguel, M. Bernien, M. Wolf, W. Kuch, P. Tegeder, J.I. Pascual, J. Am. Chem. Soc. 131 (2009) 12729.
[12] M.J. Comstock, N. Levy, A. Kirakosian, J. Cho, F. Lauterwasser, J.H. Harvey, D. A. Strubbe, J.M.J. Fr'echet, D. Trauner, S.G. Louie, M.F. Crommie, Phys. Rev. Lett. 99 (2007) 038301.
[13] C. Bronner, G. Schulze, K.J. Franke, J.I. Pascual, P. Tegeder, J. Phys.: Condens. Matter 23 (2011) 484005.
[14] P. Tegeder, J. Phys.: Condens. Matter 24 (2012) 394001.
[15] S. Seo, M. Min, S.M. Lee, H. Lee, Nat. Commun. 4 (2013) 1920.
[16] C. Bonner, B. Priewisch, K. Rück-Braun, P. Tegeder, J. Phys. Chem. C 117 (2013) 27031.
[17] T. Moldt, D. Przyrembel, M. Schulze, W. Bronsch, L. Boie, D. Brete, C. Gahl, R. Klajn, P. Tegeder, M. Weinelt, Langmuir 32 (2016) 10795.
[18] E. Fischer, Y. Hishberg, J. Chem. Soc. (1952) 4522.
[19] Y. Sueishi, M. Ohcho, N. Nishimure, Bull. Chem. Soc. Jpn. 58 (1985) 2608.
[20] N. Tamai, H. Miyasaka, Chem. Rev. 100 (2000) 1875.
[21] M. Bletz, U. Pfeifer-Fukumura, U. Kolb, W. Baumann, J. Phys. Chem. A 106 (2002) 2236.
[22] P.N. Day, Z. Wang, R. Pachter, J. Phys. Chem. 99 (1995) 9730.
[23] O. Chaudé, P. Rumpf, C.R. Acad. Sci. 236 (1953) 697.
[24] J. J. B. Flannery, J. Am. Chem. Soc. 90 (1968) 5660.
[25] R. Klajn, Chem. Soc. Rev. 43 (2014) 148.
[26] M. Furukawa, H. Tanaka, T. Kawai, J. Chem. Phys. 115 (2001) 3419.
[27] A. Riemann, B. Nelson, Langmuir 25 (2009) 4522.
[28] E. Krebs, L. Grabill, A. Riemann, Surf. Sci. 678 (2018) 143.
[29] F. Nickel, M. Bernien, K. Kraffert, D. Krüger, L.M. Arruda, L. Kipgen, W. Kuch, Adv. Funct. Mater. 27 (2017) 1702280.
[30] F. Nickel, M. Bernien, D. Krüger, J. Miguel, A.J. Britton, L.M. Arruda, L. Kipgen, W. Kuch, J. Phys. Chem. C 122 (2018) 8031.
[31] F. Neese, WIREs Comput. Mol. Sci. 2 (2011) 73.
[32] P. Bleiziffer, K. Schaller, S. Rinker, J. Chem. Inf. Model. 58 (2018) 579.
[33] X. He, V. Man, W. Yang, T.-S. Lee, J. Wang, J. Chem. Phys. 153 (2020) 114502.
[34] A. Maleki, S. Alavi, B. Najafi, J. Phys. Chem. C 115 (2011) 22484.
[35] P. Bhadra, S. Siu, Langmuir 35 (2019) 9622.

[36] W. Xiao, X. Feng, P. Ruffieux, O. Gröning, K. Müllen, R. Fasel, J. Am. Chem. Soc. 130 (2008) 8910.

[37] A.A. Starikova, B.S. Lukyanov, E.L. Mukhanov, O.A. Komissarova, G.T. Vasilyuk, S. A. Maskevich, V.I. Minkin, Russ. Chem. Bull. 67 (2018) 972.

[38] P. Sahoo, K. Prakash, S. Kumar, Supramol. Chem. 29 (2017) 183.

[39] B. Owens, A. Riemann, Surf. Sci. 624 (2014) 118.