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Self-Assembly of Molecular Landers Equipped with Functional Moieties on the Surface

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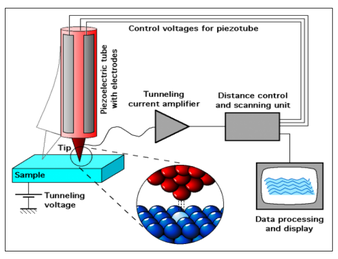
INTRODUCTION

The self-assembly of organic molecules on a metallic substrate, explored using scanning tunneling microscopy (STM), is a crucial research area in nanoscience. It relies on various interactions that are responsible for the creation of highly structured molecular arrangements, enabling precise control of the atomic-scale structure. This opens up potential applications in nanotechnology and materials science.

METHOD

1-STM(Scanning Tunneling Microscope)

Scanning Tunneling Microscopy **(STM)** a technique that images surfaces at the atomic level by measuring the tunneling current between a sharp tip and the sample.



Schematic structure of a scanning tunneling microscope

2-EHMO-ESQC:

This method was used to simulate STM (scanning tunneling microscopy) images of the self-assembled structures.

3-Molecular Mechanics Modeling (MM)

The MM4 code was used to optimize the systems on the substrate and establish nanostructures on the surface.

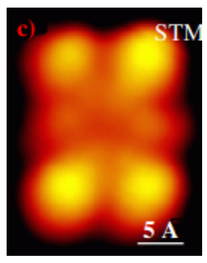
4-Ab Initio Calculations:

Conducted using the Mopac2009 code at the SCF-MP6 level to characterize the co-adsorption of molecules on the metallic substrate.

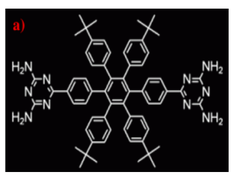
RESULTS & DISCUSSION

Adsorption of a Single Lander Molecule(DAT,DCI) on Metal Surfaces .

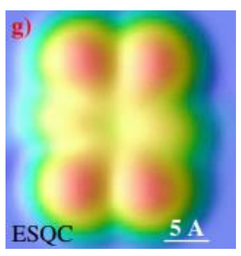
Molecule DAT:



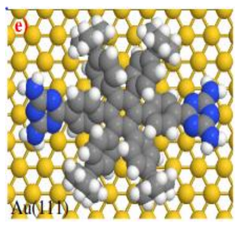
STM image



structure of molecular Lander-DAT ($C_{64}H_{68}N_{10}$)



ESQC image

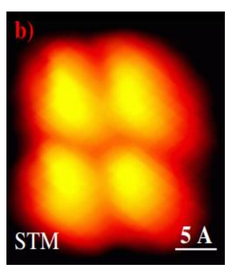


optimized chemical structure

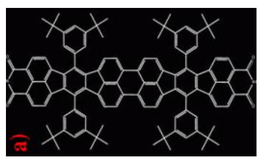
Four bright lobes in a rectangular shape,corresponding to the legs **(C_4H_9)**

of the molecule.

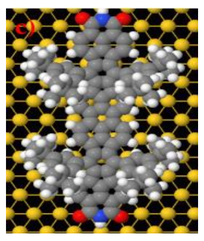
Molecule DCI:



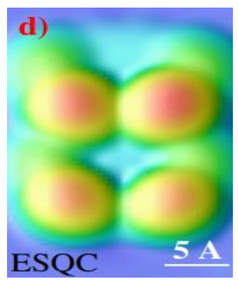
STM image



structure of molecular Lander-DCI ($C_{112}H_{102}N_2O_4$)



optimized chemical structure

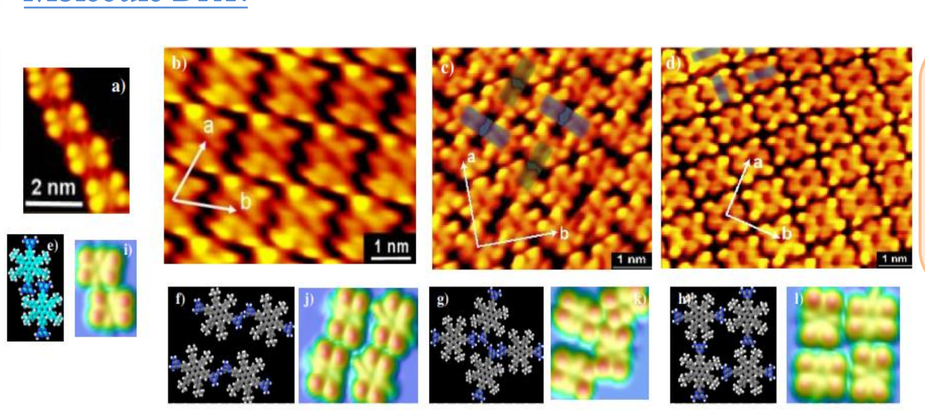


ESQC image

Four bright protrusions attributed to the four DTP legs; the central molecular board and the DCI moieties are not visible in the ESQC and STM images.

Self-Assembly Formed by Lander Molecules Guided by vdW and HB Interactions.

Molecule DAT:

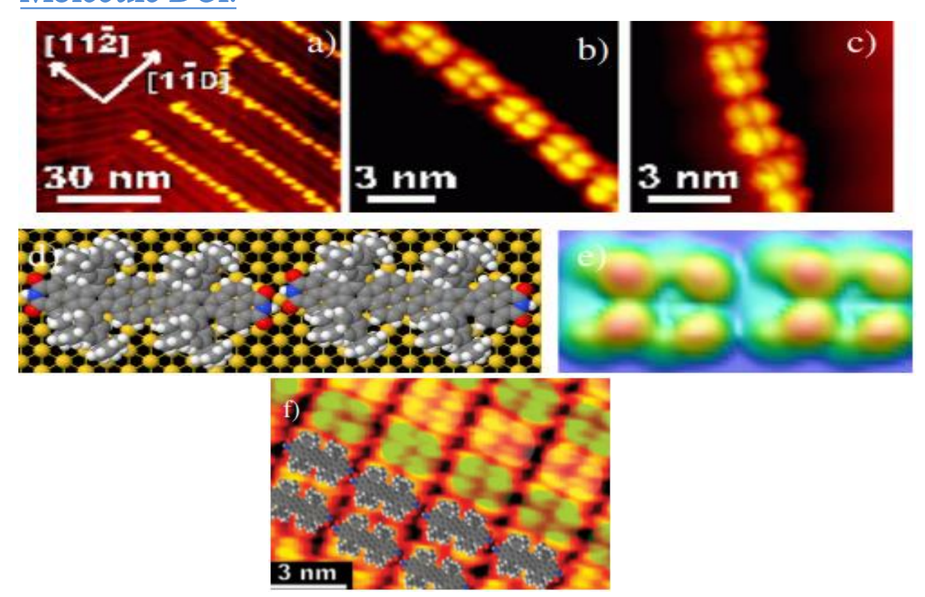


STM and Computational Analysis of Lander-DAT Nanostructures on Au(111): 1D Chains, Stripe, Four-Blade Mill, and Transition Configurations.

Distinct 2D structures were observed on the Au(111) substrate, such as ‘Four-Blade Mill’,‘Transition’, and ‘Stripe’.

An intermolecular network optimized in 3D by N - H · · · N HB.

Molecule DCI:

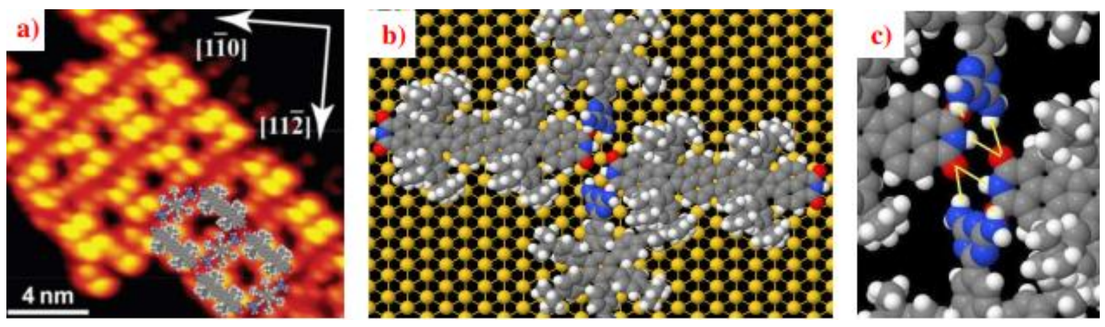


STM and Computational Study of Lander-DCI Nanostructures on Au(111): 1D Chains and 2D Networks.

The chains are connected via double N – H · · · O intermolecular hydrogen bonds. -Van der Waals interactions link the chains together.

The molecules are interconnected through double N – H · · · O hydrogen bonds

The co-adsorption of two Lander molecules, DAT and DCI, on an Au(111) surface.



STM and Computational Modeling of DAT-DCI Molecule Assembly on Au(111): 2D Structures and 3D Hydrogen Bonding.

The total energy per DAT–DCI molecular pair is higher than the total energy of DAT-DAT and DCI-DCI pairs alone (1.51 eV vs. 0.50 eV for the 2D network DCI-DCI and 0.82 eV for the 2D network DAT-DAT).

Lander-DAT molecules separate the chains by two N – H · · · O HBs (2.66 Å and 3.46 Å), between the DAT group and DCI group in Lander-DCI molecules.

CONCLUSION

The self-assembly of Lander molecules through non-covalent interactions, showing that co-adsorption can create stable structures via hydrogen bonding, van der Waals forces, and electrostatic interactions. The stronger 3D hydrogen bonding in heteromolecular networks highlights the potential for developing new nanostructures on various substrates for nanotechnology.

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