Molecular Architectures and electronic properties of 5,14-ol-5,14-diborapentacyclo on noble metal surfaces

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In recent studies [1, 2], heteroatoms-doped precursors have frequently been used to polymerize graphene nanoribbons with a large variety of structures or dopant heteroatoms. Using cryogenic scanning tunneling microscopy, we investigated the structure of self-assembled 5,14-ol-5,14-diborapentacyclo (CM218) on Cu(110), Cu(111), and Ag(111). While the order is relatively poor on Cu(110) where only few molecular chains can be observed for the second molecular layer, much better ordered molecular clusters and two-dimensional islands are found on Cu(111) at very low and medium sub-monolayer coverage, respectively.

The main focus of our study, though, is on CM218 on Ag(111), where we find that molecular clusters and chains coexist with molecular islands. Topographic images of these honeycomb structures display a pronounced bias dependence. Molecule-functionalized tips allow for high-resolution images of these structures for which we suggest structural models. We investigate the electronic properties by scanning tunneling spectroscopy and differential conductance mapping.

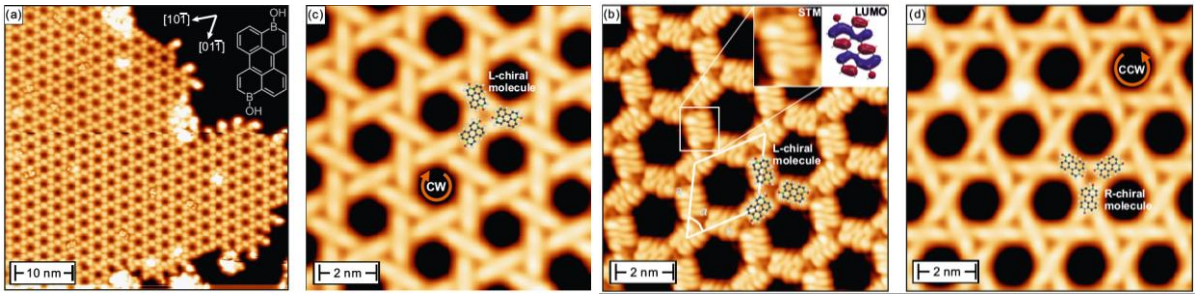

Fig. 1. (a) STM topography of 5,14-ol-5,14-diborapentacyclo (DBPTCD) on Ag(111). (b) Zoom-in image (a) with a molecular functionalized tip shows the molecular orbital shape of the Kagome supramolecular structure. Inset is the comparison of STM topography and DFT calculated LUMO. (c,d) STM topographies of two typical Kagome supramolecular structure areas found on the same sample of (b), Scanning parameters: (a) U = +1.0 V, I = 100 pA; (b) U = -100 mV, I = 300 pA; (c) U = -1.0 V, I = 500 pA; (d) U = -1.0 V, I = 800 pA (sample bias).

[1] Q. Zhong *et al*., Nature Chemistry **13**, 1133 (2021)
[2] K. Sun *et al*., Nature Chemistry **15**, 136 (2023)