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On-Surface Synthesis of Novel π-Magnetic Materials

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On-surface synthesis (OSS)[1] paved the way for fabricating polyaromatic hydrocarbons (PAH) exhibiting magnetism.[2] Such magnetic properties may arise from unpaired π-electrons, which may either be stabilized by π-conjugation (resonance & aromaticity arguments) or simply due to an odd number of π electrons. Herein, we present two examples of π-magnetic PAHs fabricated by OSS and characterized by scanning tunneling microscope & spectroscopy (STS) and DFT.

First, we present the OSS of PAH based on acenes, known to have open-shell characters: A pentacene-based precursor resulted in various fused dimers. (Figure 1) Bond-resolving (BR) STM revealed the structures of the products while STS and DFT calculations revealed that the closed- or open-shell character were dependent on the fusion motif, rationalized by (anti-)aromatic character of the central ring.

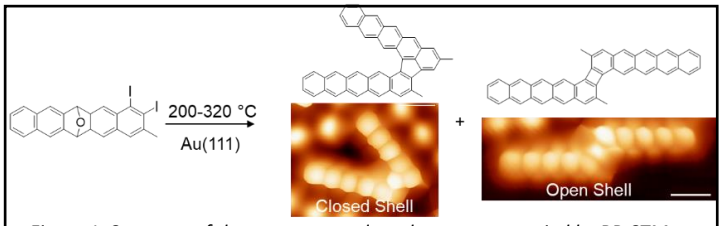

Figure 1. Structure of the precursor and products accompanied by BR-STM.

Second, we report the OSS of an N-doped triangulene, a PAH having an odd number of π-electrons. OSS from a ketone-based derivative followed reduction and annealing, resulting in Aza-Triangulene (AzaT).[3] BR-STM confirmed the structure of the target product. (Figure 2) STS revealed that the electronic properties and magnetic fingerprints (Kondo resonance) point to charge transfer in both directions, illustrating how the substrate may also influence the magnetic properties of the material.[3] Further annealing of the material on both substrates resulted in fused derivatives that display various magnetic states.

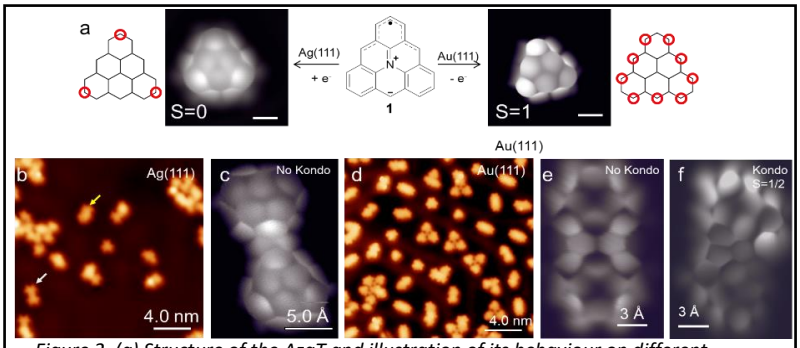

Figure 2. (a) Structure of the AzaT and illustration of its behaviour on different substrates. Large scale STM images of Fusion products on (b) Ag(111) and (c) Au(111) and BR-STM images of selected products.

Thus, this presentation provides insight into the molecular design, characterization techniques, electronic structure, and possible future applications of carbon-based magnetic materials.

Références

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