Parameters Inhibiting the Growth of Nanoporous Graphene from PAH Molecules in Favor of Metal–Organic Network

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The on-surface bottom-up synthesis of nanostructured graphene, such as graphene nanoribbons (GNRs) and nanoporous graphenes (NPGs), offers precise control over electronic properties, ranging from semimetals to semiconductors, making these materials promising candidates for applications in flexible nanoelectronics and quantum computing. This synthesis typically involves a two-step reaction route induced by annealing and the catalytic behaviour of the metallic substrate. The growth of nanostructured graphenes depends primarily on the molecular precursor used, which tailors the architecture of the final product (1).

In this study, we initially investigated how the shape of the precursor and the position of halogen substitutions in the intact powder of a triphenylene-based molecule influence its vibrational and electronic properties through a combined experimental and DFT approach. The molecule was then deposited and studied under ultra-high vacuum (UHV) conditions on Au(111) and Ag(111) substrates using scanning tunnelling microscopy (STM) operated at room temperature. This molecule serves as a potential precursor for the NPG elaboration via a two-step on-surface reaction. However, due to geometric confinement and steric hindrance between neighbouring molecules, the dehalogenated precursors are unable to approach closely enough to form C–C covalent bonds. As a result, the initial reaction step – i.e., Ullmann coupling - is suppressed, favouring the formation of metal–organic networks instead (see Figure 1).

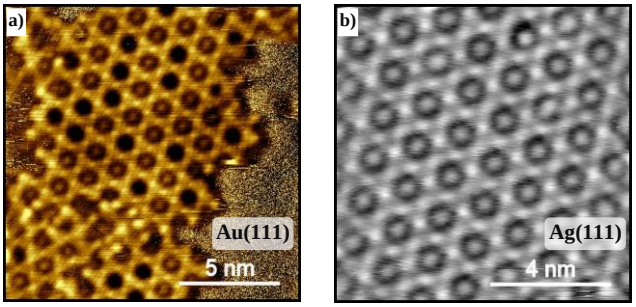

Figure 1: *RT-STM images of metal-organic network formed by triphenylene derivative on Au(111) and Ag(111) surfaces held at 100 °C and 150 °C, respectively. Scanning parameters: (a) 15x15 nm², V_b = 1.7 V, I_t = 7 pA; (b) 10x10 nm², V_b = -2.0 V, I_t = 10 pA.*

REFERENCES

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