

On Surface Synthesis of graphite-N-doped Molecular Graphene Nanostructures

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Graphene and its derivatives have been widely investigated with the exotic electronic properties. Doping is one of the most important ways to tune the properties of graphene-based nanostructures and materials.

The π -conjugated di- and polyradicals is attractive as a designable platform to explore the molecules spin interaction and development of organic magnetic materials. The introduction of graphite-N is one of most promising way to realize the construction of the π -conjugated polyradicals platforms. here we present the construction of an NHC-derived 1,3,5-TMB (N-TMB). In the target N-TMB molecule, the TMB core is stabilized by three NHC modules, which are further fused by benzene rings to the backbone with the expectation of improving the stability and spin coupling of the triradical. The N-TMB exhibits threefold symmetry on Au(111) and is structurally verified by nc-AFM techniques. STS characterization combined with DFT calculations reveals the occurrence of strong charge transfer between N-TMB and the substrate, resulting in positively charged N-TMB³⁺ on Au(111) surface. We further design and synthesize other N-doped 0D and 1D molecular graphene nanostructures and exploit their electronic structures.

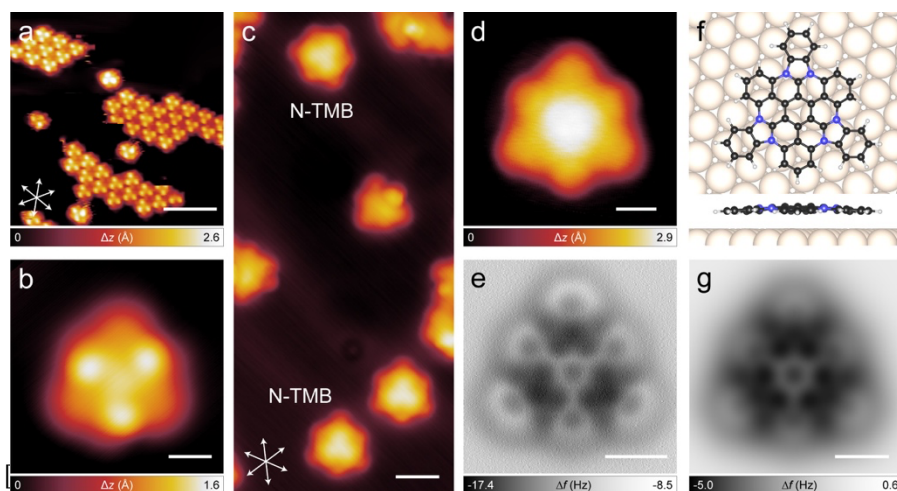


Figure 1 On-surface synthesis of N-TMB on Au(111).

1. J.-J. Duan; X.-Q. Yang; R. Li; X. Li; T. Chen; D. Wang. *J. Am. Chem. Soc.* 2024, 146, 19, 13025.

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