Heterotriangulene Kagome Graphene Films: Growth and Effect of Kinetic Reaction Parameters

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Nanoporous graphenes (NPGs) featuring Kagome lattices formed by heterotriangulene (HT) units continue to attract interest for their correlated electronic properties. Their symmetry gives rise to flat bands, and recent experimental work demonstrates the ability to introduce defects resulting in local magnetic moments [1–3]. Covalent organic frameworks (COFs) such as these are often synthesized through surface-assisted Ullmann coupling on a coinage metal substrate, and thus are susceptible to defects such as missing units, irregular-sided linkages, and limited grain sizes of around 100 nm [4,5]. The problem of reduced dimensionality and lack of a reversible, self-correction mechanism within COF networks pose a continuing challenge for defect-free synthesis. Additionally, limited empirical growth data make finding optimal growth parameters nontrivial.

To clarify the evolution of HT precursors into ordered NPGs, we perform a series of direct polymerization growths over a range of sample temperatures (180–250 °C) and deposition rates for tribromo- and triiodotrioxaazatriangulene (TBTANG and TITANG) precursors on Au(111). Using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) we interrogate how deposition conditions and choice of halogen affect the final polymer film quality, which we quantify using minimum spanning tree and persistent homology approaches [6]. We also investigate the prevalence of halogenated edge terminations and occurrence of undesired organometallic intermediates. Experimental results are complemented by kinetic Monte Carlo simulations as well as simulated STM and nc-AFM analyses. By mapping the kinetic reaction parameter space, we establish the basis for more complex structures such as lateral 2D heterojunctions with HTs of differing bridge groups. Such structures may exhibit robust optoelectronic properties as seen in their hole-conductive triphenylamine counterparts.

Reference

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