Sulfur-doped Graphene Nanoribbons with a Sequence of Distinct Band Gaps

SHI-XUAN DU, YAN-FANG ZHANG, YI ZHANG, Institute of Physics, Chinese Academy of Sciences, REINHARD BERGER, Max Planck Institute for Polymer Research, XINLIANG FENG, Technische Universitt Dresden, KLAUS MULLEN, Max Planck Institute for Polymer Research, XIAO LIN, Institute of Physics, Chinese Academy of Sciences, YU-YANG ZHANG, SOKRATES T. PANTELIDES, Vanderbilt University, HONG-JUN GAO, Institute of Physics, Chinese Academy of Sciences — Unlike free-standing graphene, graphene nanoribbons (GNRs) can possess semiconducting band gap. However, achieving such control has been a major challenge in the fabrication of GNRs. Chevron-type GNRs were recently achieved by surface-assisted polymerization of pristine or N-substituted oligophenylene monomers. By mixing two different monomers, GNR heterojunctions can in principle be fabricated. Here we report fabrication and characterization of chevron-type GNRs by using sulfur-substituted oligophenylene monomers to achieve GNRs and related heterostructures for the first time. Importantly, our first-principles calculations show that the band gaps of GNRs can be tailored by different S configurations in cyclodehydrogenated isomers through debromination and intramolecular cyclodehydrogenation. This feature should open up new avenues to create multiple GNR heterojunctions by engineering the sulfur configurations. These predictions have been confirmed by Scanning Tunneling Microscopy (STM) and Scanning Tunneling Spectroscopy (STS). The unusual sequence of intraribbon heterojunctions may be useful for nanoscale optoelectronic applications based on quantum dots.

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