Molecular Bandgap Engineering in Bottom-Up Fabricated Graphene Nanostructures

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Abstract:

Bandgap engineering has long played a vital role in technology by enabling semiconductor heterostructures to exhibit important behaviors such as resonant tunneling and enhanced solar conversion efficiency. As the dimensions of conventional electronic devices reduce further in size, however, their performance suffers due to short-channel effects and rough interfaces. Graphene-based molecular electronics has emerged as a possible candidate to overcome these obstacles by enabling control of electronic transport down to single-molecule scales. Graphene nanoribbons (GNRs), for example, exhibit bandgaps that can be readily modified by tuning their width and symmetry, and electronic components based on single-layer GNRs featuring widths smaller than 2 nm have been demonstrated. It has been predicted that bandgap engineering within single GNRs may be achieved by varying the width of covalently bonded GNR segments, but the experimental realization remains challenging. We demonstrate the rational bottom-up synthesis of width-modulated armchair GNR (AGNR) heterostructures, obtained by fusing segments of two different molecular building blocks. We study the resultant heterojunctions at sub-nanometer length-scales via scanning tunneling microscopy (STM) and spectroscopy (STS), and identify spatially modulated electronic structure that demonstrates molecular-scale bandgap engineering. First-principles calculations support our experimental findings and provide further insight into the microscopic electronic structure of bandgap-engineered GNR heterojunctions.