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Structure and Electronic Properties of Polymer Chains and Graphene Nanoribbon Formed by Molecular Self-Assembly on Au(111).

CHUANXU MA, MIGUEL A. FUENTES-CABRERA, BOBBY G. SUMPTER, KUNLUN HONG, AN-PING LI, Oak Ridge National Laboratory, ZHONGCAN XIAO, WENCHANG LU, J. BERNHOLC, North Carolina State University — Graphene nanoribbons (GNRs) with bandgaps are promising building blocks for ultra-fast electronics. Bottom-up synthesis of GNRs from aromatic hydrocarbon molecules has been proven to be an effective way to control GNR's width with atomically precise edge structures. Using scanning tunneling microscopy (STM), we study the formation of both linear polymer chains and narrow GNRs in the bottom-up self-assembly process with the DBBA molecules as the precursor on Au(111). The linear polymer chains are formed after the deposition of DBBA and 200 C annealing for 30 min. The polymers can be converted to 7-AGNRs (seven-carbon wide armchair GNRs) after 400 C annealing. Interestingly, second-layer polymer is seen to survive on the GNRs during the annealing process. This result indicates that the Au(111) substrate plays an important role in the dehydrogenation process and the formation of GNRs, which is confirmed by our DFT calculations. Electronically, the polymers show a bandgap of 3.4 eV, much larger than that of GNRs. After annealing at 500 C for 30 min, wider GNRs can form: 14-AGNR, 21-AGNR. The 7-AGNR shows a typical edge state at -1.1 eV, while for 14-AGNR it is at -1.35 eV. Moreover, junctions of GNRs with different widths can be formed with pronounced boundary states.

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