

Abstract Submitted  
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**Ab initio study of the mechanism of bottom-up synthesis of graphene nanoribbons** ZHONGCAN XIAO, North Carolina State University, CHUANXU MA, HONGHAI ZHANG, LIANGBO LIANG, JINGSONG HUANG, Oak Ridge National Laboratory, WENCHANG LU, North Carolina State University, KUNLUN HONG, AN-PING LI, Oak Ridge National Laboratory, JERRY BERNHOLC, North Carolina State University — Graphene nanoribbons (GNRs) can be fabricated with atomic precision by using molecular precursors deposited on a metal substrate, and potentially form the basis for future molecular-scale electronics. The precursor molecules are first annealed to form a polymer, and further annealing at a higher temperature leads to the formation of a GNR. We systematically study the reaction pathways of this cyclodehydrogenation process, using density functional theory and the nudged elastic band method. We find that the Au substrate reduces the reaction barriers for key steps in the cyclodehydrogenation process: cyclization, hydrogen migration and desorption. Furthermore, our calculations explain recent experiments showing that an STM-tip can induce local polymer-to-GNR transition, which can be used to fabricate atomically precise heterojunctions: at a negative bias, the STM tip injects excess holes into the polymer HOMO state, lowering the energy barrier in agreement with Woodward-Hoffmann rules. At a positive bias, when excess electrons are injected into the LUMO state, the energy barrier is not significantly lowered and the transition is not observed.

Zhongcan Xiao  
North Carolina State University

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