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Kinetic Pathways towards Fabrication of Narrow Graphene Nanoribbons on Stepped Metal Surfaces[1] PING CUI, JIN-HO CHOI, Univ. of Sci. and Tech. of China, HUA CHEN, Univ. of Tennessee, Univ. of Texas at Austin, WEI CHEN, Univ. of Tennessee, WENGUANG ZHU, Univ. of Tennessee, Oak Ridge National Lab, CHANGGAN ZENG, Univ. of Sci. and Tech. of China, ZHENYU ZHANG, Univ. of Sci. and Tech. of China, Harvard University — Graphene nanoribbons (GNRs) are predicted to exhibit intriguing electronic transport properties that strongly depend on their widths. To this end, one standing challenge is controlled fabrication of narrow GNRs with sizeable band gaps. In this study, we use first-principles approaches to explore the possibility of growing narrow GNRs along the step edges of catalytic metal surfaces. By minimizing the lattice mismatches of the growing graphene islands, optimizing their adsorption geometries, and exploiting the diffusion anisotropy of selective precursor monomers on the stepped surfaces, we identify the growth conditions under which the precursor monomers can be nucleated at the steps and then grow along the steps. Our studies point to kinetic pathways towards controlled fabrication of some of the narrowest GNRs with zigzag or armchair edges, and are expected to stimulate experimental efforts to realize these predictions.

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