Structure and Electronic Properties of Polymer Chains and Graphene Nanoribbon Formed by Molecular Self-Assembly on Au(111)
submitted by Dr. Chuanxu Ma, with ID 61213787, and this talk following Dr. Ma's?
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Computational study of bottom-up fabrication of armchair graphene nanoribbons ZHONGCAN XIAO, North Carolina State University, CHUANXU MA, MIGUEL FUENTES-CABRERA, Oak Ridge National Lab, WENCHANG LU, North Carolina State University; Oak Ridge National Lab, ANPING LI, KUNLUN HONG, JINGSONG HUANG, BOBBY SUMPTER, Oak Ridge National Lab, JERRY BERNHOLC, North Carolina State University; Oak Ridge National Lab — Graphene nanoribbons have promising electronic properties for nanotechnology. They can be fabricated using a bottom-up procedure with specific molecular precursors, which results in atomically precise nanoribbon structures. Herein we demonstrate the formation of a 7-atomic-layer pristine armchair graphene nanoribbon from the 10,10'-dibromo-9,9'-bianthracene precursor through polymerization followed by cyclodehydrogenation. We performed calculations using density functional theory with van der Waals corrections to study how Au(111) and Cu(111) substrates affect the energy profiles for the reaction process. To further understand the effects of the substrate on the cyclodehydrogenation procedure, we also considered double-layer ribbon structure on top of the substrate. These results may provide insight into the use of different precursors for producing both polymers and ribbons with novel electronic properties.

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