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Surface-assisted formation of graphene nanoribbons on Au surfaces CLAUDIA CARDOSO, DEBORAH PREZZI, ELISA MOLINARI, ANDREA FERRETTI, S3 Center, Istituto Nanoscienze, CNR via Campi 213/A, 41125, Modena, Italy — The formation of graphene nanoribbons (GNRs) on Au(110) and Au(111), as based on the surface-mediated reaction of 10,10′-dibromo-9,9′ bianthracene (DBBA) molecules was investigated by means of first-principles calculations. The study was done in direct collaboration with experimental groups performing structural and spectroscopic characterization by means of STM, XPS/UPS, NEXAFS. Comparison between the Au(110) and Au(111) surfaces unveils the delicate interplay between surface atomic corrugation, molecular mobility, and adsorption energies, that drive the GNR growth. Concerning the Au(110) surface, we have studied the molecule/surface interaction at different stages of the GNR formation. The role of different reconstructions has been investigated, showing that both precursors and GNRs interact differently with different surfaces. Calculations for the precursor molecules showed that initial stages of the reaction crucially determine the final configuration and orientation of the GNRs. In the specific case of Au(111) we have also studied the evolution of the Au Shockley surface state as a function of GNR growth. We show that the GNR/Au interaction results in an upshift of the Shockley surface state of Au(111) by 0.2 eV, together with an increased electron effective mass.

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