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Role of Au surface step edge on bottom-up growth of atomically precise graphene nanoribbons: First-principles study[1] TOMOAKI KANEKO, NOBUO TAJIMA, TAKAHISA OHNO, National Institute for Materials Science — The formation of energy gap in graphene can be understood as a critical problem for graphene electronic device application. One of the way to introduce the band gap is use of graphene nanoribbons (GNR). Especially, the bottom-up growth can produce high quality and atomically precise armchair GNR, but their length is limited up to few tens nm. For the GNR growth, 10,10′-dibromo-9,9′-bianthryl (DBBA) precursor molecules polymerize on Au surface at 470 Kelvin and resultant poly-anthracene becomes into GNR by surface assisted cyclodehydrogenation at 670 Kelvin. In order to obtain much longer GNR, understanding of the formation of poly-anthracene is necessary. In this study, we investigated the adsorption of DBBA, poly-anthracene and GNR on Au surfaces by means of first-principles calculations using PHASE code. The effect of van der Waals interaction was included by the semi-empirical method by Grimme. To discuss the effect of surface morphology, we considered the flat Au(111) and stepped Au(443). We found that DBBA and poly-anthracene are stable at the step edges. These results should be an origin of recently reported growth of spacially aligned GNR on Au(887) stepped surfaces.

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