Supplementary Information

Long and Oriented Graphene Nanoribbon Synthesis from Well-ordered 10,10'-Dibromo-9,9'-Bianthracene Monolayer on Crystalline Au Surfaces

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Figure S1. Processed image of Figure 1a. The contrast caused by DBBAs was removed by Fourier transform filtering to highlight the buried Au(111)-herringbone reconstruction structure. Blue lines represent the ridges of herringbone reconstruction.



monolayer heating method on Au(111) (a) and Au(100) (b). The green dots in the inserted images show the positions where Raman spectroscopy measurements were performed on each Au substrate. The grey areas represent the positions where components were attached to hold the substrates.



Figure S3. Schematic images of intermolecular distance before and after GNR synthesis. The lattice constant of GNR is based on the report by Q. Wang *et al.*.[1]

		GNR coverage (%)		
	Calculation			
	<i>D_{DBBA}</i> (Å)	(D _{GNR} /D _{DBBA)}	STM result	
on Au(111)	18	49	52±1	
on Au(100)	14	63	67±2	

Table S1. Change in intermolecular distance and coverage before and after GNR synthesis.



Figure S4. STM image around well-ordered DBBA submonolayer and Au(100)-hex boundary ($V_S = 2.0$ V, $I_T = 100$ pA). The observed DBBA supply for submonolayer fabrication is 65% of that for monolayer fabrication. Inset molecular image shows the adsorption position of DBBA molecules.

Table S2. The adsorption energy of benzene on Au(111) and Au(100) by theoretical calculations. PBE, RPBE, and RevPBE are DFT calculations using Perdew-Burke-Ernezerhof functionals. D3 and 3D(ABC) mean empirical dispersion correction. BJ means employing Becke-Johnson exchange potential.

[2] W. reckien <i>et al.</i>	$E_{ads}(kJ/mol)$		
	benzene/Au(111)	benzene/Au(100)	
PBE-D3	-83	-87	
PBE-D3(BJ)	-84	-89	
PRBE-D3	-84	-85	
RevPBE-D3	-105	-103	
RevPBE-(BJ)	-121	-123	
PBE-D3(ABC)	-70	-74	
[3] Y. Jiang <i>et al.</i>	$E_{ad}(kJ/mol)$		
	benzene/Au(111)	benzene/Au(100)	
PBE+vdW ^{sruf}	-72.4	-78.2	
PBE+MBD	-54.0	-62.7	
PBE	0.96	-8.68	
MBD	-55.0	-54.0	

References

- [1] Wang et al., J. Phys. Chem. C, 2021, 125, 6034–6042
- [2] W. Reckien et al., J. Org. Chem., 2014, 10, 1775–1784.
- [3] Y. Jiang et al., Sci Rep, 2016, 6, 39529.