Electronic Supplementary Material (ESI) for Nanoscale

Intrinsic Electronic and Transport Properties of Graphyne Sheets and Nanoribbons

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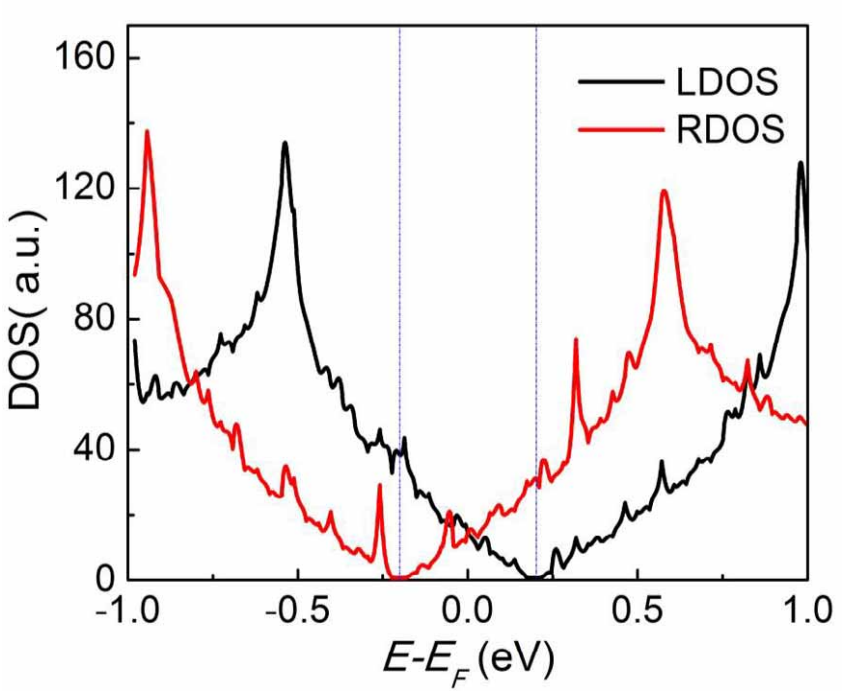

Figure S1. Density of states (DOS) of the left (LDOS) and right (RDOS) electrodes under the bias voltage of 0.4 V for the two-probe α-graphyne device. The chemical potentials of left and right electrodes (u_L and α u_R) are separated by eV_b = 0.4 eV.

Table S1. Relative total energies of ferromagnetic (FM), antiferromagnetic (AFM), and nonmagnetic (NM) states of a ZGyNR.

(N_{a1}; N_{a2})	E_{NM}-E_{FM} (meV)	E_{NM}-E_{AFM}(meV)
8-α-ZGyNR	31	34
4-β-ZGyNR	2	9
5-β-ZGyNR	7	44.7
4-γ-ZGyNR	0	0
6-γ-Z'GyNR	67.5	102.3
6-6,6,12-ZGyNR	32	50

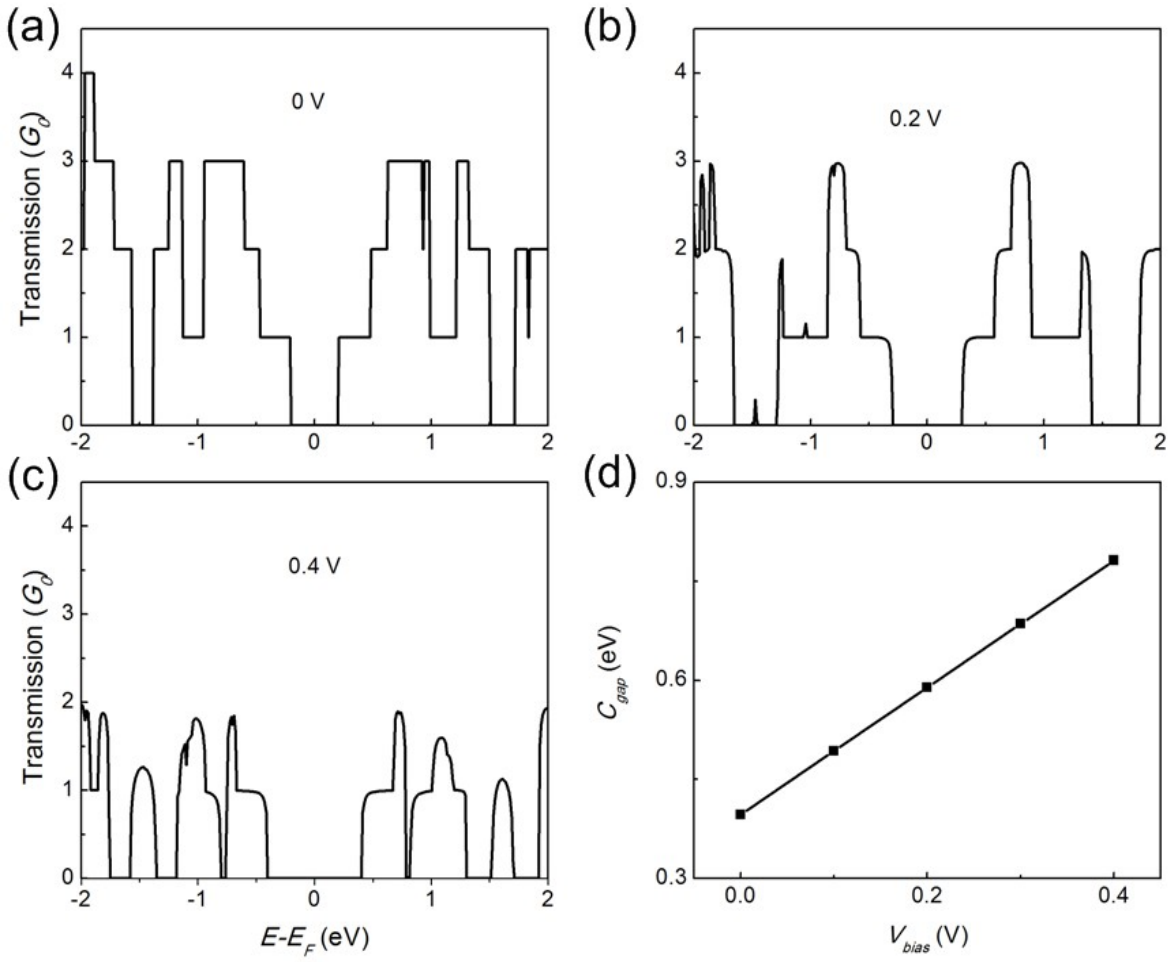

Figure S2. Computed transmission spectra of 6-α-AGyNR under the bias voltages of (a) 0.0, (b) 0.2, and (c) 0.4 V, respectively. (d) The variation of the conductance gap C_{gap} as a function of bias voltage.

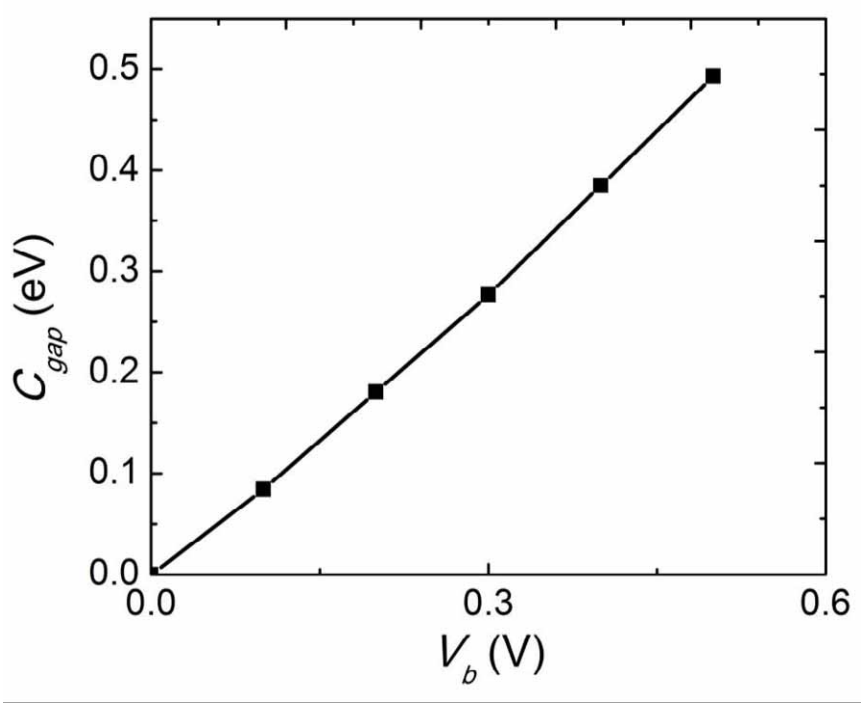

Figure S3. The variation of the conductance gap C_{gap} as a function of bias voltage for the 6-α-ZGyNR.

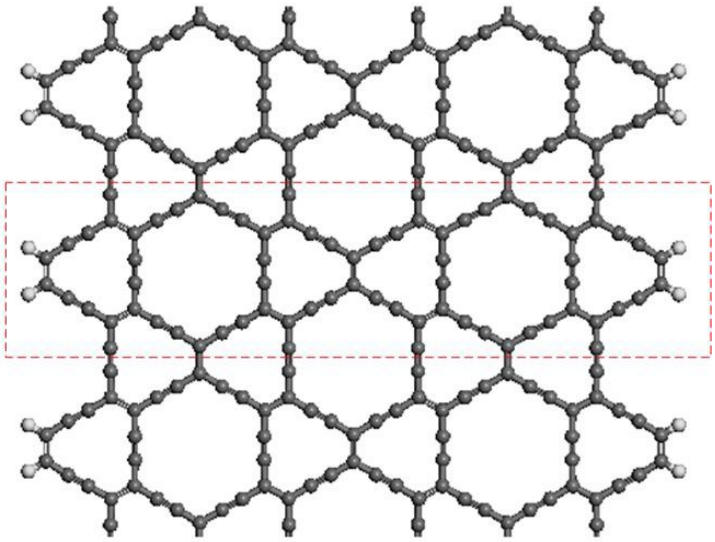

Figure S4. The optimized atomic structure of 2-β-AGyNR. The gray and white balls denote C and H atoms, respectively. The dashed rectangle denotes the unit cell of 2-A-β-graphyne NR.

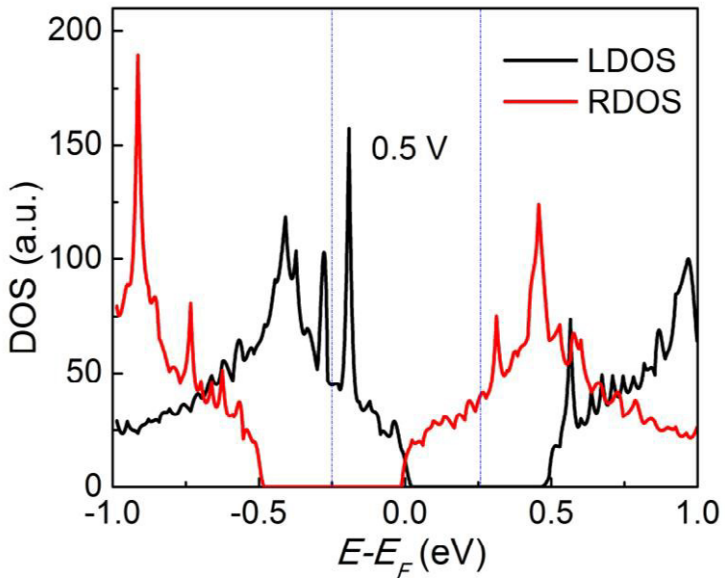

Figure S5. Density of states (DOS) of the left (LDOS) and right (RDOS) electrodes under the 0.5 V bias voltage for the two-probe γ-graphyne sheet device. The chemical potentials of left and right electrodes (u_L and u_R) are separated by eV_b = 0.5 eV.

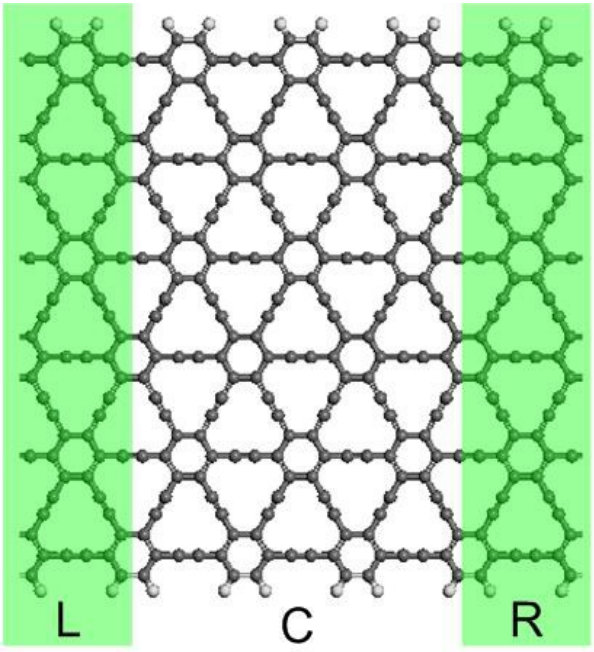

Figure S6. Schematic view of the two-probe 6-γ-AGyNR device.