Supplemental Information: Curvature in graphene nanoribbons generates temporally and spatially focused electric currents

C. G. Rocha,[1,2] R. Tuovinen,[1] R. van Leeuwen,[1] and P. Koskinen[1]

[1] *Nanoscience Center, Department of Physics, University of Jyväskylä, 40014 Jyväskylä, Finland*
[2] *School of Physics, Trinity College Dublin, Dublin 2, Dublin, Ireland*

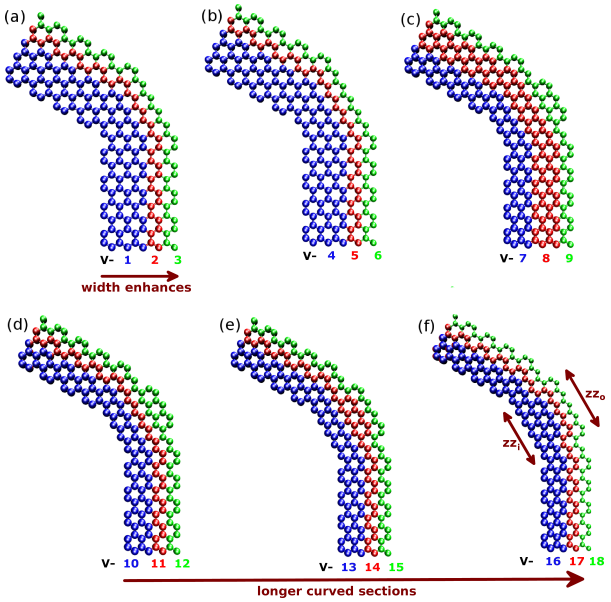

FIG. 1: (Color online) Systematic set of curved graphene nanoribbon (CGNR) samples with 60° angles. There are three different widths (blue thinnest, red intermediate, and green widest) for each type of curvature. Notation for each sample is given at the bottom of each panel: (a) V-1, V-2, V-3; (b) V-4, V-5, V-6; (c) V-7, V-8, V-9; (d) V-10, V-11, V-12; (e) V-13, V-14, V-15; (f) V-16, V-17, V-18. Their structural information, including the number of zigzag segments at the inner (zz_i) and outer (zz_o) edges, are shown in Table I. All samples are hydrogen-terminated, but hydrogens are omitted from the figures for clarity. The samples discussed in the main text are V-2 (sample V_a) and V-18 (sample V_b).

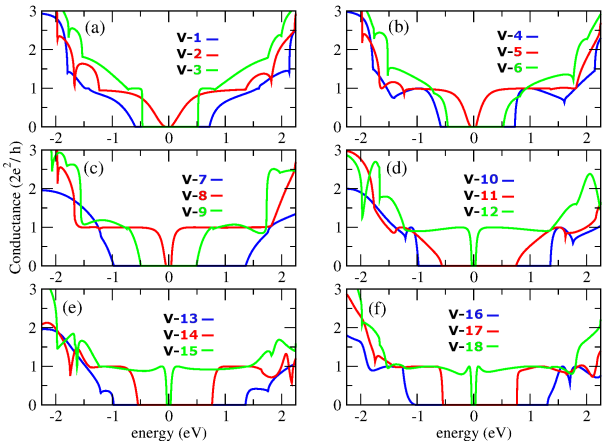

FIG. 2: (Color online) Conductance as a function of energy for all CGNRs of Fig. 1 (using corresponding ordering).

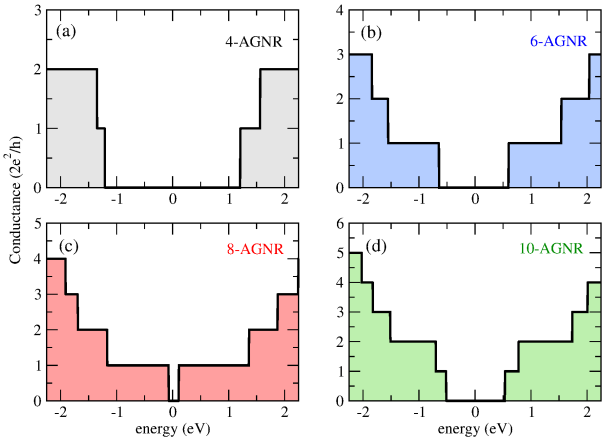

FIG. 3: (Color online) Conductance as a function of energy for straight armchair graphene nanoribbons of width N =4, 6, 8, 10.

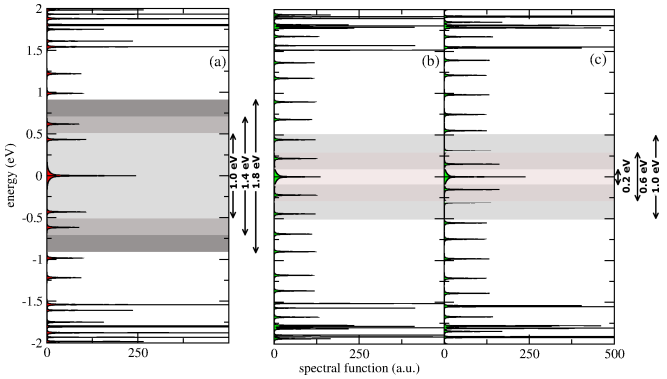

FIG. 4: (Color online) Spectral function for the (a) V-2 (sample V_a in main text), (b) V-9, and (c) V-18 (sample V_b in main text) CGNRs. Fermi energy is at 0 eV. Gray areas span the relevant energy ranges at different biases, to better identify the possible states involved in transitions.

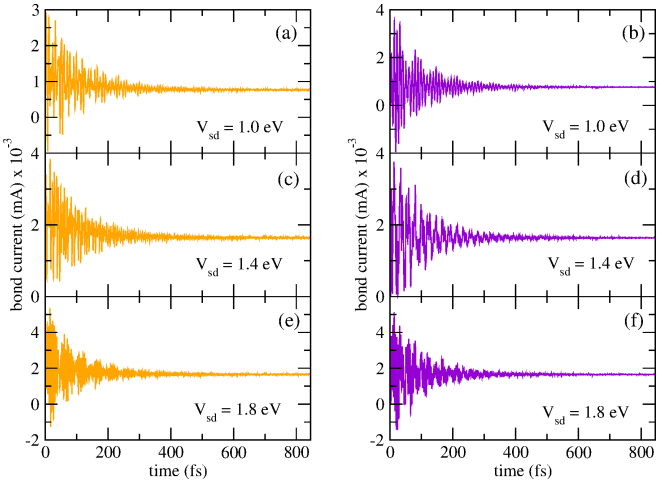

FIG. 5: (color online) Long-time currents through V-2 CGNR (sample V_a in main text) at bridge B1 (left panels) and at bridge B2 (right panels), using bias voltages V_{SD} = 1.0, 1.4, and 1.8 eV (top to bottom panels).

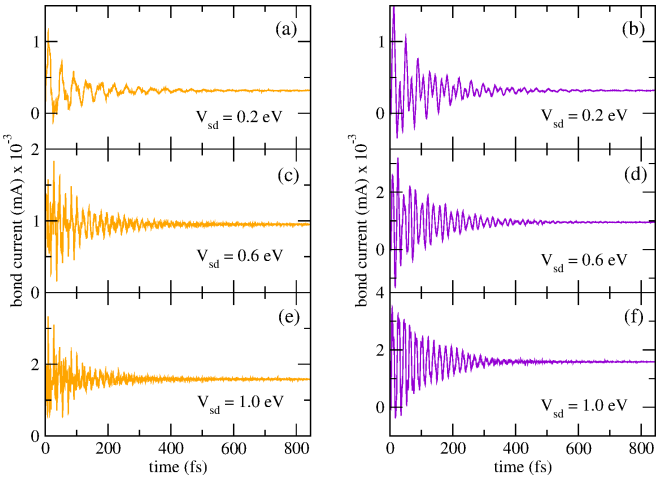

FIG. 6: (color online) Long-time currents through V-9 CGNR at bridge B1 (left panels) and at bridge B2 (right panels), using bias voltages $V_{\rm SD} = 0.2$, 0.6, and 1.0 eV (top to bottom panels).

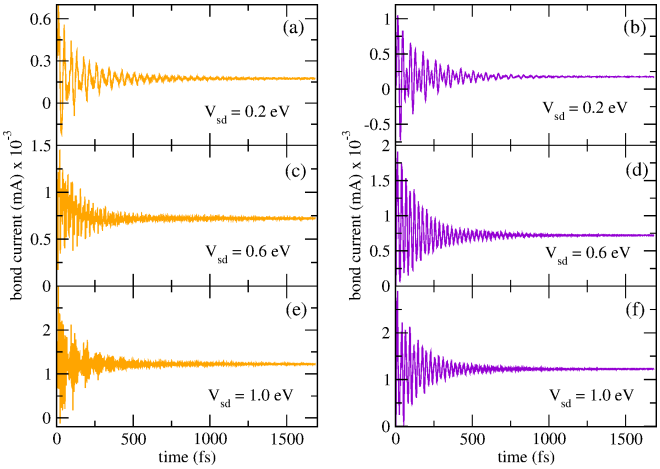

FIG. 7: (color online) Long-time currents through the V-18 CGNR (sample V_b in main text) at bridge B1 (left panels) and at bridge B2 (right panels), using bias voltages $V_{\rm SD} = 0.2$, 0.6, and 1.0 eV (top to bottom panels).

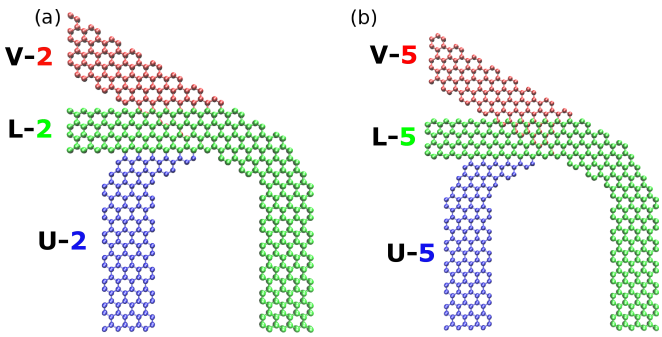

FIG. 8: (Color online) Set of CGNR samples with 90° (green) and 180° (blue) angles, in addition to the familiar 60° (red) angle. (a) CGNRs V-2 (sample V_a in main text), U-2 (sample U in main text), and L-2 (sample L in main text) have short curved parts. (b) CGNRs V-5, U-5, and L-5 have longer curved parts. All samples are hydrogen-passivated, but the hydrogens are omitted from the figure for clarity.

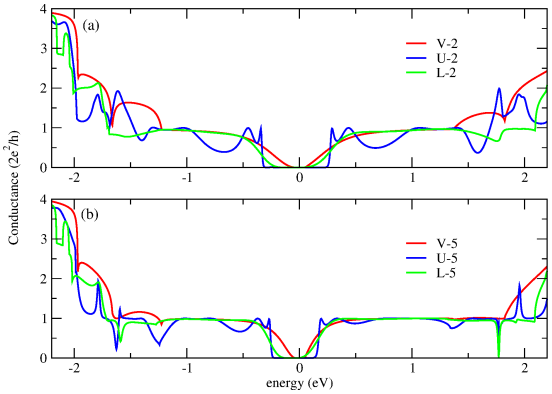

FIG. 9: (Color online) Conductance as a function of energy for the CGNRs shown in Fig. 8.

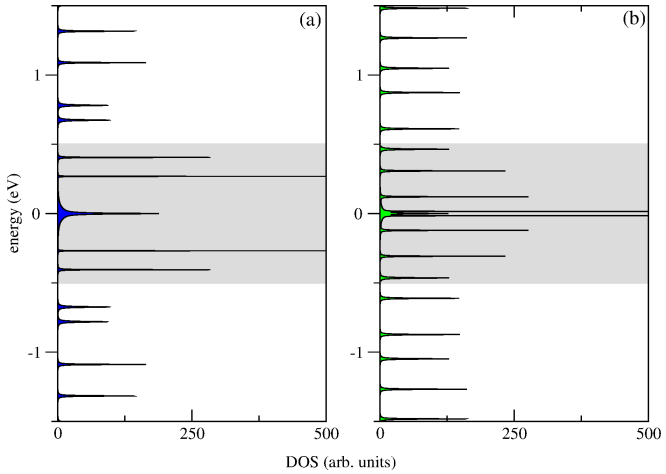

FIG. 10: (Color online) Spectral function for the (a) U-2 (sample U in main text) and (b) L-2 (sample L in main text) CGNRs. Fermi energy is at 0 eV. Gray areas span the relevant energy ranges at different biases, to better identify the possible states involved in transitions.

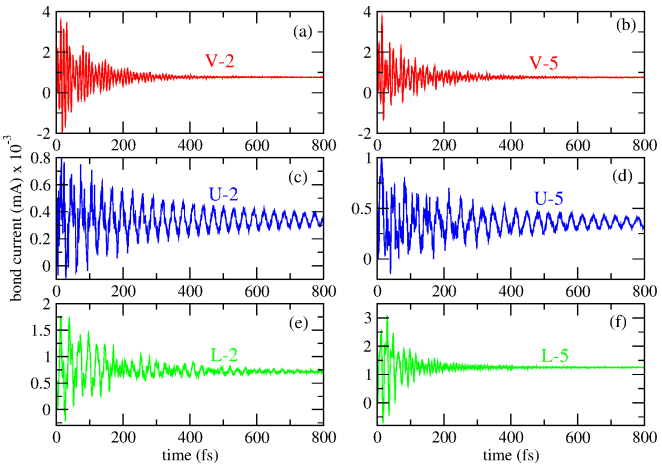

FIG. 11: (color online) Long-time currents through the CGNRs (a) V-2, (b) V-5, (c) U-2, (d) U-5, (e) L-2, and (f) L-5 at bias $V_{SD} = 1.0$ eV. Currents are measured at bridges in the middle of the curved section.

TABLE I: Structural parameters of the V-junctions shown in Fig. 1: number of zigzag segments in the inner (zz_i) and outer (zz_o) edges, number of armchair segments located in the outer curved edge (ac), lead type (GNR) and its width (W), inner (R_i) and outer (R_o) mean radius of curvature, and the mean width of the curved part ($W_c = R_o$ - R_i).

V-junctions								
Label	zz_i	zz_o	ac	GNR	W (Å)	R_i (Å)	R_o (Å)	W_c (Å)
V-1	0	4	0	6-AGNR	6.12	11.80	16.20	4.40
V-2	0	6	0	8-AGNR	8.57	11.80	18.40	6.60
V-3	0	8	0	10-AGNR	11.02	11.80	20.62	8.82
V-4	2	6	0	6-AGNR	6.12	14.01	18.40	4.39
V-5	2	8	0	8-AGNR	8.57	14.01	20.62	6.61
V-6	2	10	0	10-AGNR	11.02	14.01	22.84	8.83
V-7	4	6	0	4-AGNR	3.67	16.02	18.41	2.39
V-8	4	10	0	8-AGNR	8.57	16.02	22.84	6.82
V-9	4	8	2	10-AGNR	11.02	16.02	25.95	9.93
V-10	6	8	0	4-AGNR	3.67	18.42	20.62	2.20
V-11	6	10	0	6-AGNR	6.12	18.42	22.84	4.42
V-12	6	8	2	8-AGNR	8.57	18.42	25.90	7.48
V-13	8	10	0	4-AGNR	3.67	20.64	22.84	2.20
V-14	8	8	2	6-AGNR	6.12	20.64	25.91	5.27
V-15	8	10	2	8-AGNR	8.57	20.64	28.27	7.63
V-16	10	8	2	4-AGNR	3.67	22.65	25.86	3.21
V-17	10	10	2	6-AGNR	6.12	22.65	28.23	5.58
V-18	10	12	2	8-AGNR	8.57	22.65	30.57	7.92