SUPPLEMENTARY INFORMATION

Reconstruction of the symmetry between sublattices: A strategy to improve the transport properties of edge-defective graphene nanoribbon transistor

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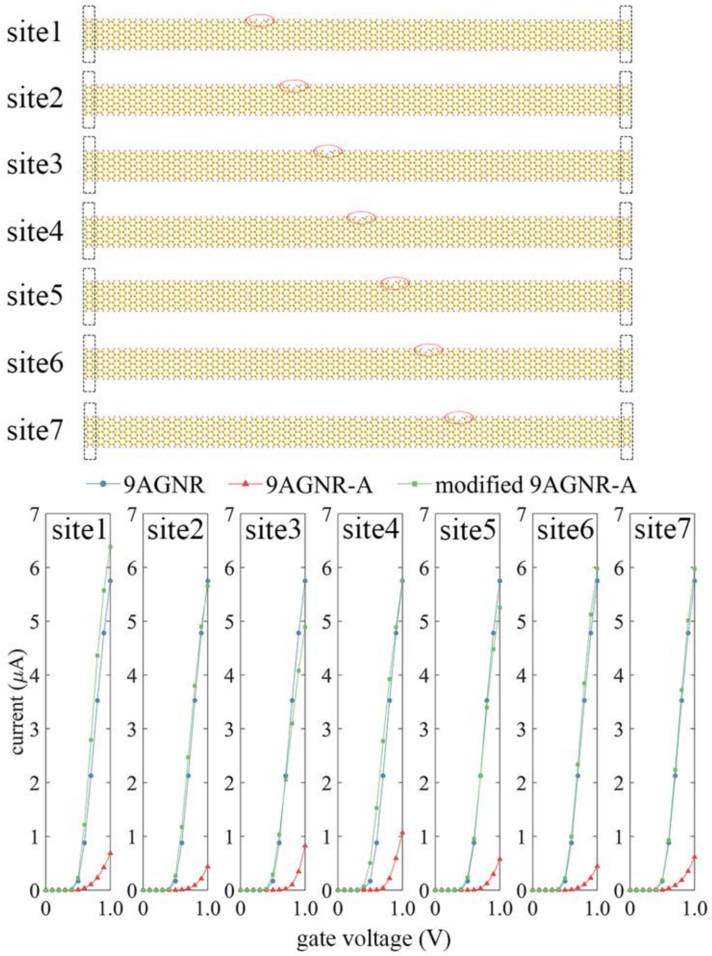

Fig. S1 9AGNR-A devices with edge defect located at different sites and corresponding transfer characteristic curves. Although the currents of different 9AGNR-A devices are different, all 9AGNR-A devices show obvious degraded performances compared to perfect 9AGNR device. More importantly, all modified 9AGNR-A devices show better performances than corresponding 9AGNR-A devices, and their performances are very close to perfect 9AGNR device. Therefore, our modified strategy is effective for arbitrary edge defect location.

To analysis the relative energy stability of modified structures respect to other ribbons, we adopt the edge formation-energy per length defined as:

$$\varepsilon_{\mathrm{H}_2} = \frac{1}{2L}\left(E^{\mathrm{ribb}} - N_{\mathrm{C}}E^{\mathrm{bulk}} - \frac{N_{\mathrm{H}}}{2}E_{\mathrm{H}_2}\right),$$

where E^{ribb}, E^{bulk}, and $E\mathrm{H}_2$ are the total energy of the ribbon supercell, of one atom in "bulk" graphene and of the isolated H_2 molecule. N_{C} (N_{H}) is the number of carbon (hydrogen) atoms in the ribbon supercell. L is the length of the ribbon. We select 10AGNR and 12ZGNR (which manifests zigzag edges and has a similar width to 10AGNR) as the references. The edge formation-energy table is shown below.

	10AGNR	12ZGNR	modified 10AGNR -A	modified 10AGNR -B	modified 10AGNR -D	modified 10AGNR -E	modified 10AGNR -F	modified 10AGNR -G	modified 10AGNR -H
ε_{H_2}(eV/Å)	0.048	0.122	0.029	0.006	0.025 (0.025)	0.051 (0.053)	0.032	0.029	-0.009

As there are two possible final modified structures for 10AGNR-D and 10AGNR-E, thus two edge formation-energies corresponding to them are shown in the table. All modified systems manifest the lower edge formation-energy than 12ZGNR. Modified 10AGNR-E shows the slightly higher edge formation-energy than 10AGNR. The rest modified structures show the lower edge formation-energy than 10AGNR. The lower edge formation-energy means the more stable structure. Therefore, all the modified structures are more stable than 12ZGNR, and most of them are more stable than 10AGNR, while modified 10AGNR-E are slightly less stable than 10AGNR.

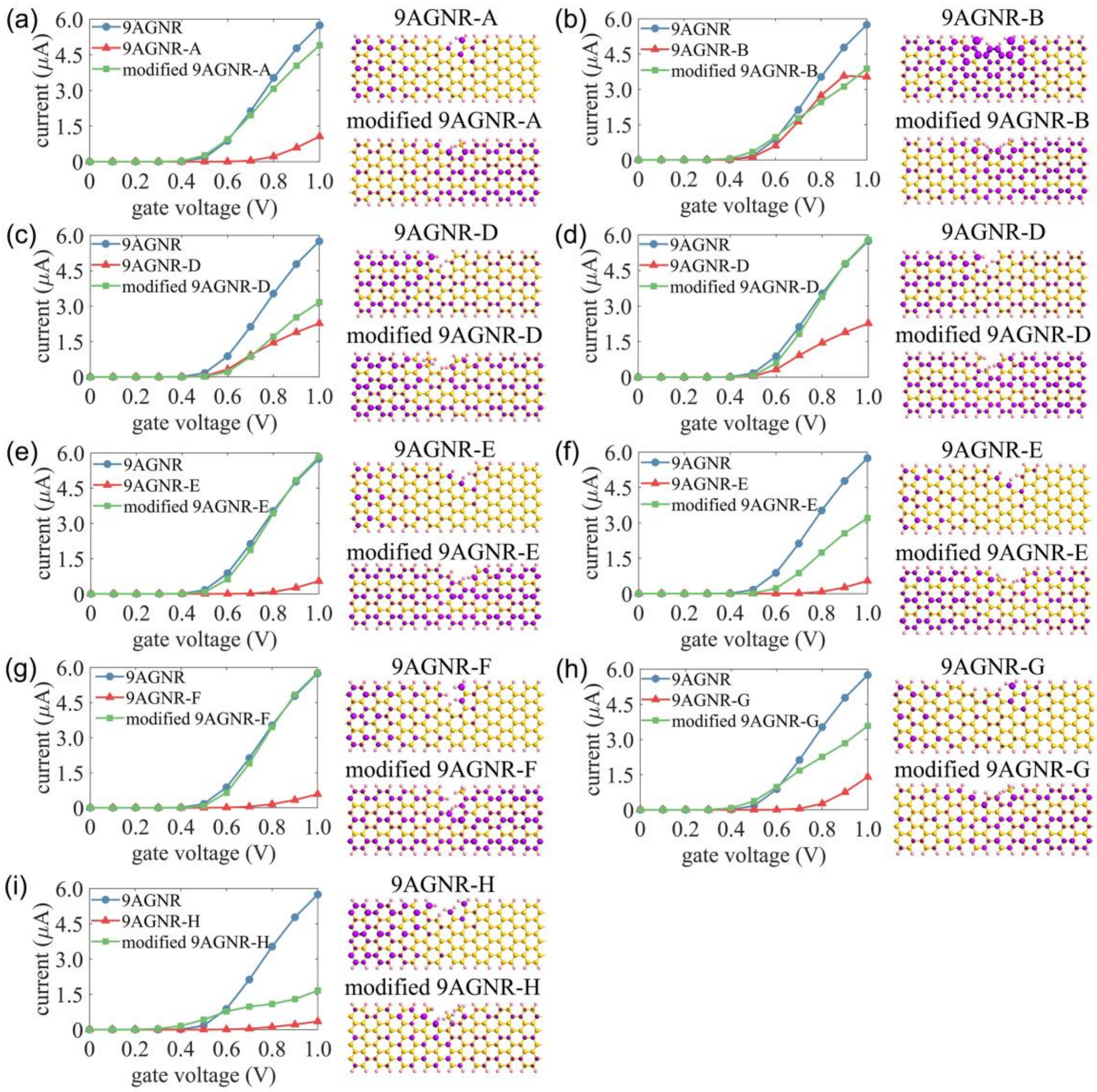

Fig. S2 The transfer characteristic curves and the transmission eigenstates at V_{GS} = 1.0 V of defective and modified 9AGNR devices. The improvement effects are similar to 10AGNR systems except that modified 9AGNR-B and modified 9AGNR-G show improved performances, whereas modified 10AGNR-B and modified 10AGNR-G do not show significantly improved performances.

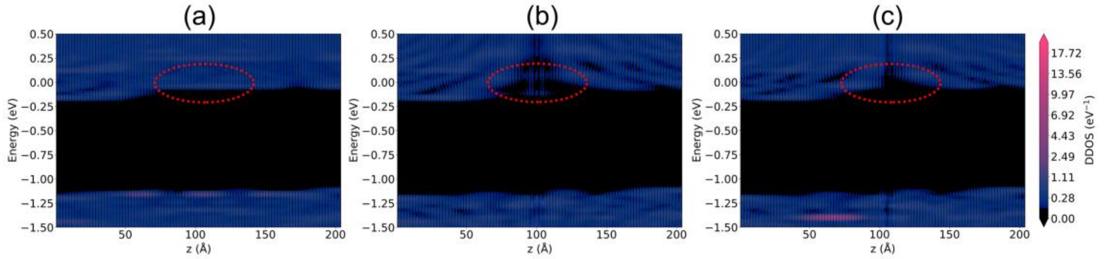

Fig. S3 The real-space device density of states (DDOS) of perfect 10AGNR, modified 10AGNR-B and modified 10AGNR-G devices at V_{GS} = 1.0 V. It can be observed that there are DDOS gaps for both modified 10AGNR-B and modified 10AGNR-G systems, while the DDOS of perfect 10AGNR are undamaged.

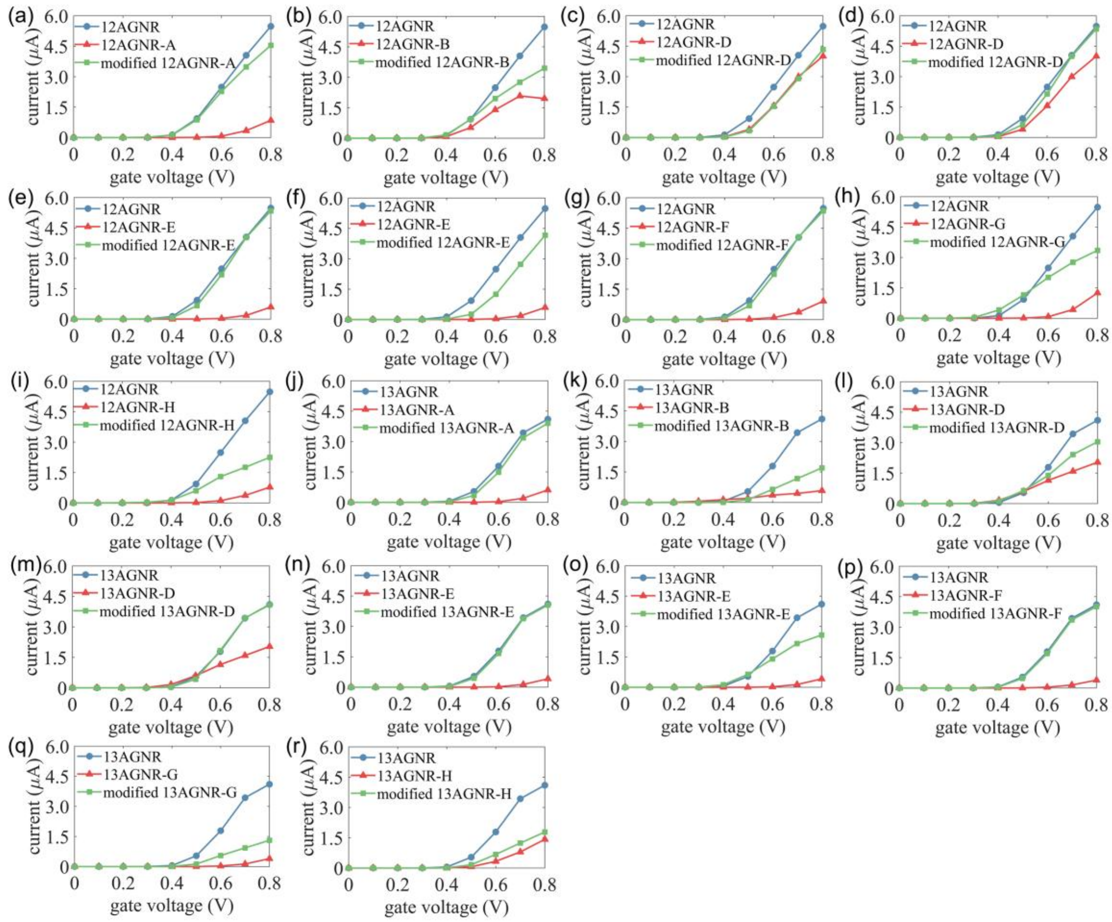

Fig. S4 The transfer characteristic curves of perfect, defective and modified 12AGNR and 13AGNR devices.