Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Intrinsic electronic and transport properties of graphene nanoribbon with different widths

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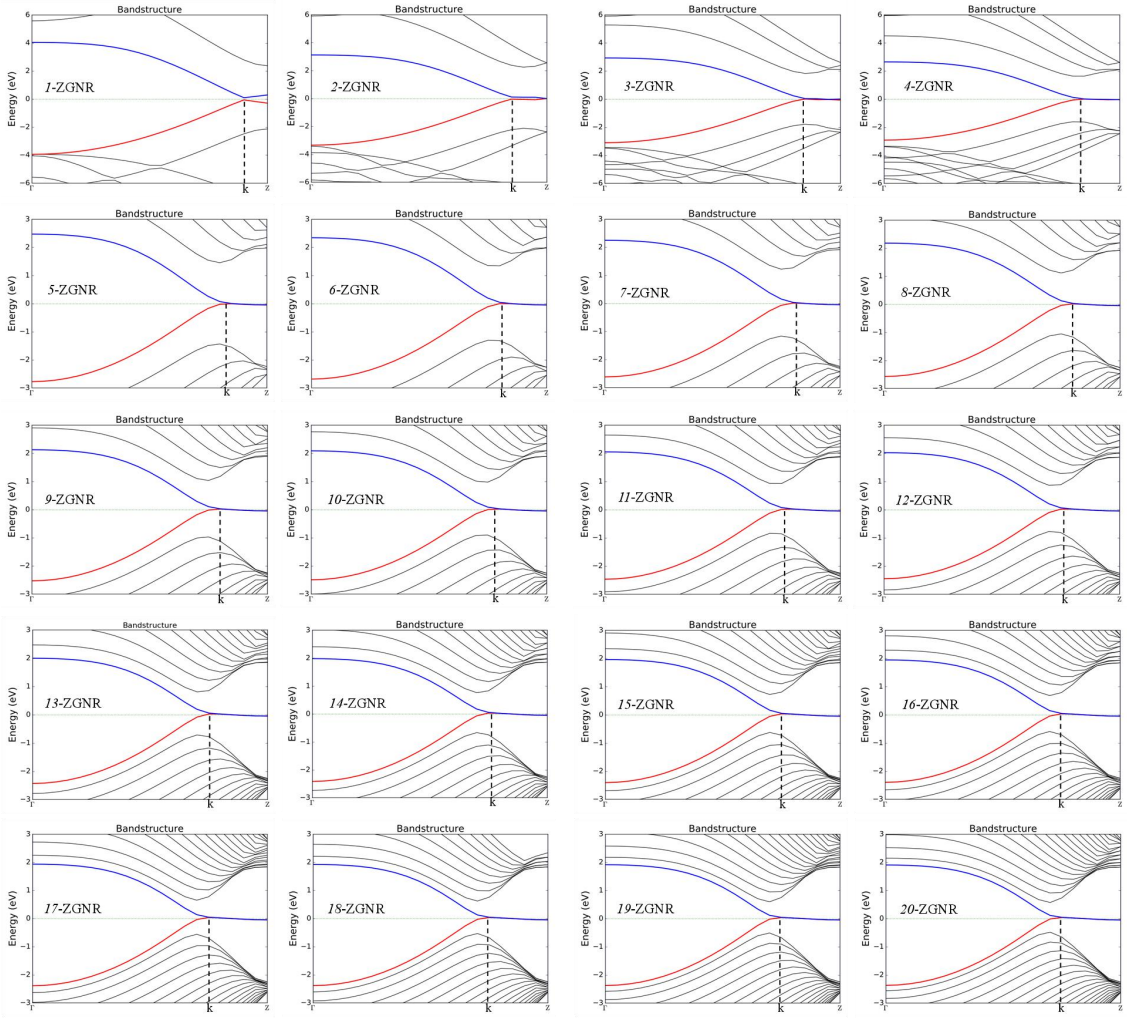
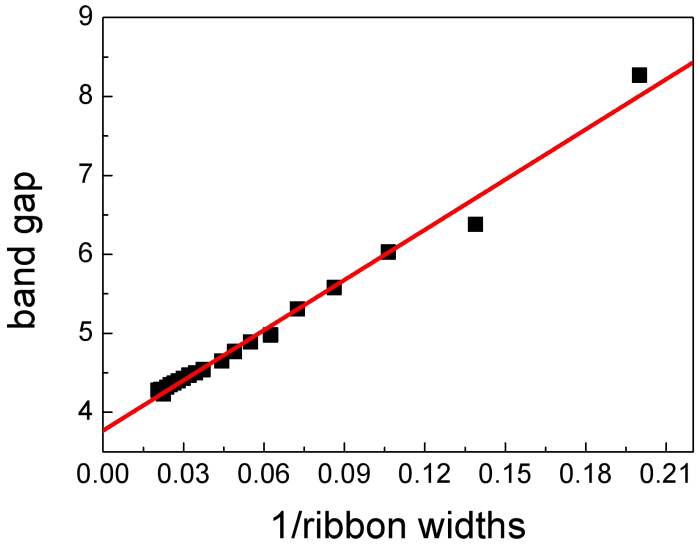


SI-1 The band structures of all calculated models.

SI-1 shows the band structures of all calculated models. In the manuscript, only several representative samples have been given. Here, the band structures of all calculated models are compiled together for comparison. As we have seen, the lowest conduction and the highest valence bands are getting closer from Γ to K, and they become degenerated finally at the K point in the Brillouin zone. However, with increasing the ribbon width, the band gap formed by the highest valence bands and the lowest conduction bands at Γ point decreases.

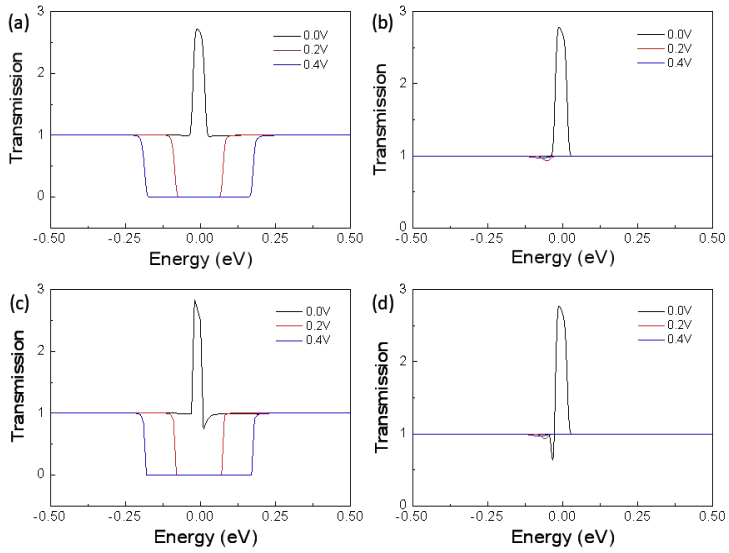


SI-2 The band gap of n-ZGNR as a function of the reciprocal of the ribbon widths.

The linear relationship between the band gap and the reciprocal of the ribbon widths has been presented in **SI-2**. The red line corresponds to the mathematical fitting with the following equation:

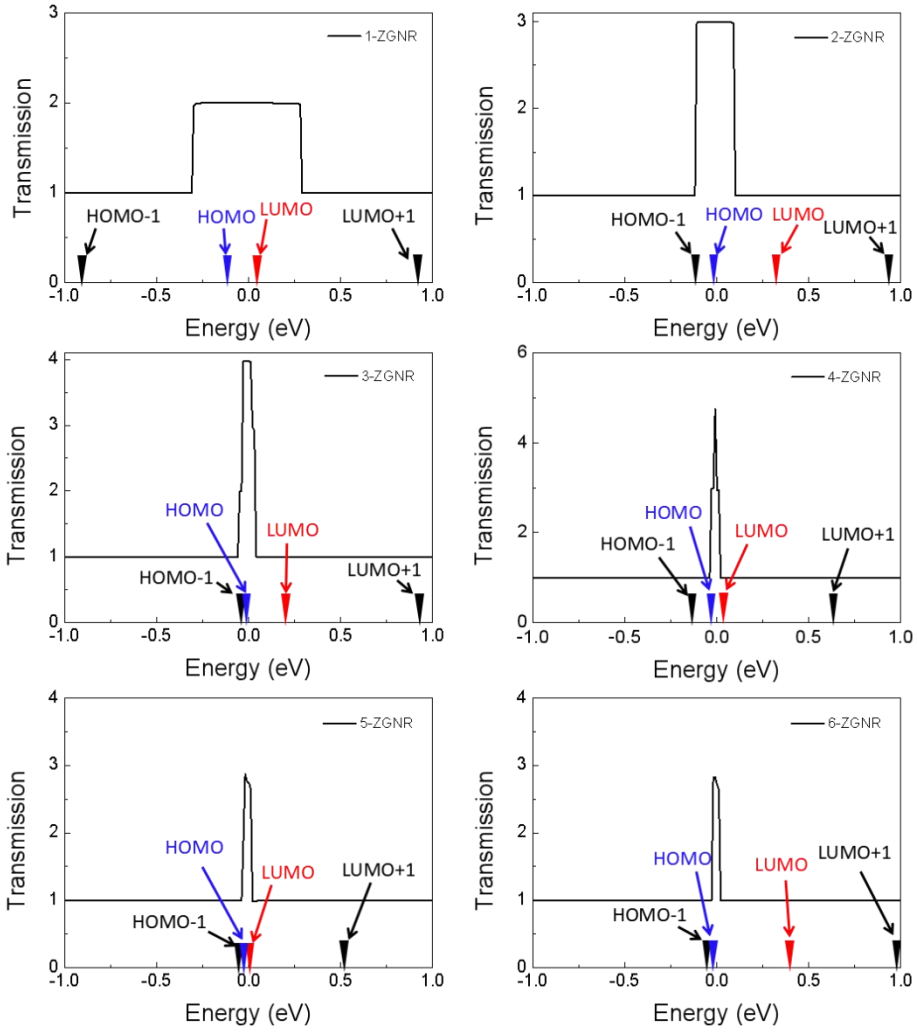
$$G = 21.2 \times \frac{1}{W} + 3.8$$

The band bap corresponding to the infinite width, i.e., the graphene, is 3.8 eV.



SI-3 Transmission spectra of (a) *7*-ZGNR, (b) *8*-ZGNR, (c) *9*-ZGNR, (d) *10*-ZGNR at different bias.

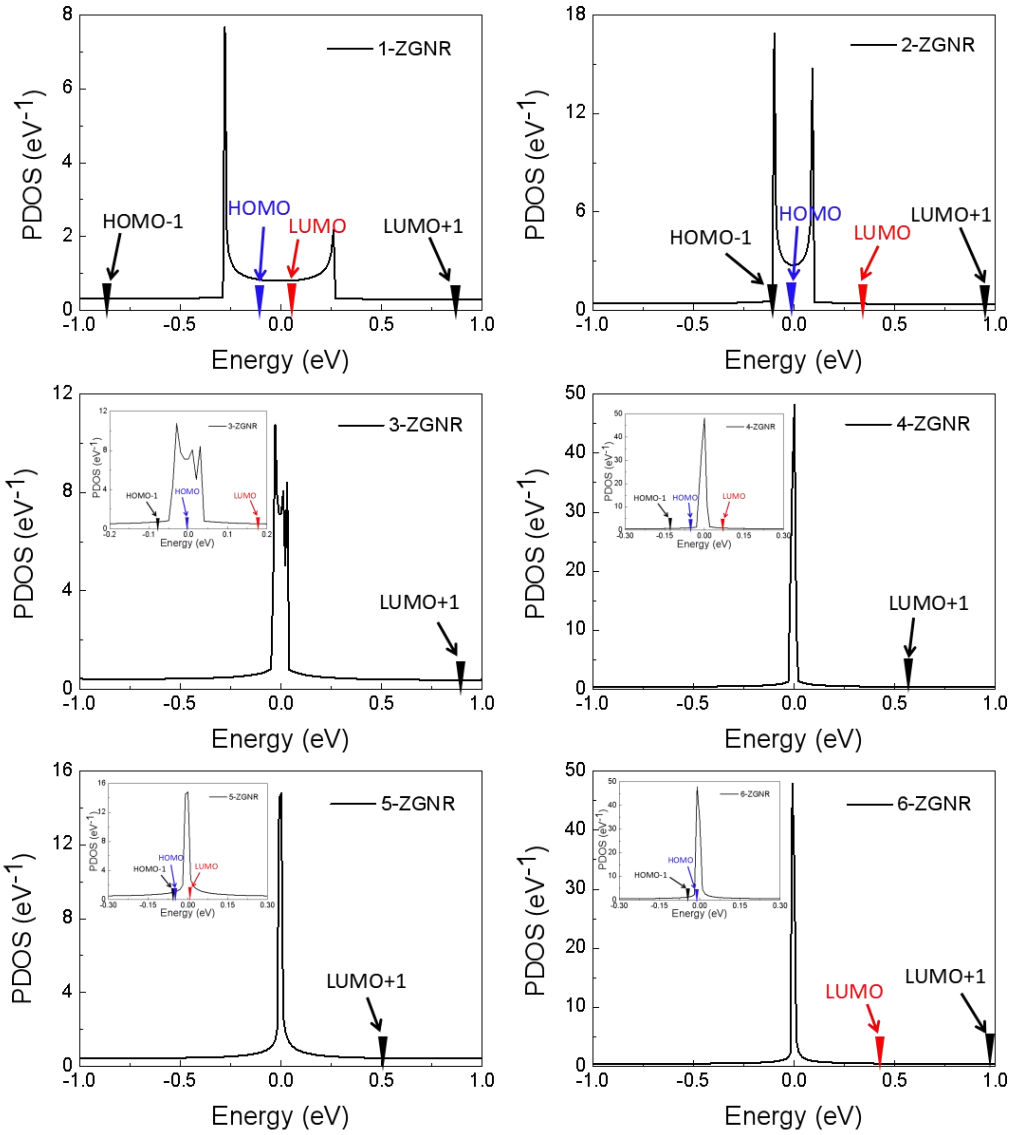
In the manuscript, only several typical models (from *1*-ZGNR to *6*-ZGNR) have been presented. Other broader models behave in the exactly same manner, as given in **SI-3**. For the odd nanoribbon, when the bias is applied, the transmission peak near the Fermi level rapidly drops to zero, forming the blocking region of the electron transfer. With increasing the bias, the energy range of the blocking region becomes wider. As for the even samples, *8*-ZGNR and *10*-ZGNR for example, there is a sharp transmission peak at zero bias. When a higher bias is applied, this transmission peak near the Fermi level drops rapidly, and its value reaches to 1. Therefore, there is at least one effective electron transport channel regardless of the applied bias.



SI-4 The transmission spectra of *n*-ZGNR ($1 \le n \le 6$) at zero bias.

As shown in **SI-4**, all models have a transmission peak near the Fermi level at

zero bias. For narrow ZGNRs ($1 \leq n \leq 3$), a rectangular shape wave is observed in a certain energy range. As the ZGNR becomes wider, the rectangular transmission wave becomes narrow, and then, it turns a sharp peak, which is contributed by the HOMO.

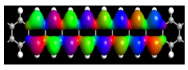
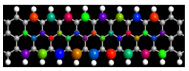
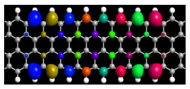
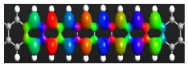
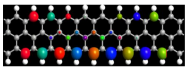
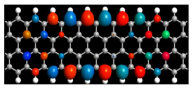
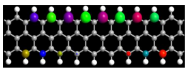


SI-5 The projected density of states (PDOS) of *n*-ZGNR ($1 \leq n \leq 6$).

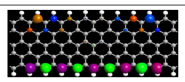
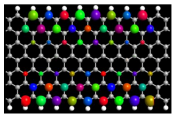
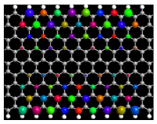
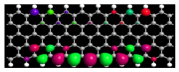
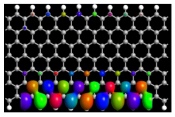
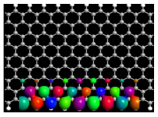
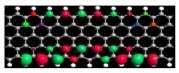
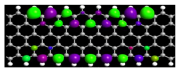
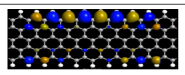
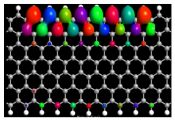
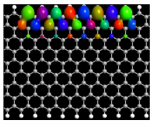
As shown in the **SI-5** that gives the positions of HOMO-1, HOMO, LUMO and LUMO+1. It should be noted that the PDOS peaks of *1*-ZGNR, *2*-ZGNR and *3*-ZGNR are localized at -0.28, -0.12, and -0.03 eV, respectively. With careful analysis of the positions of the molecular orbitals, these peaks are mostly contributed by HOMO or HOMO+LUMO. And the PDOS plots for the rest of nanoribbons, they

have only one peak around the Fermi level, which is contributed by the HOMO.

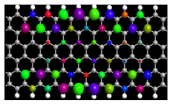
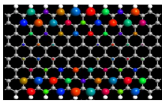
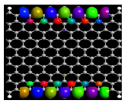
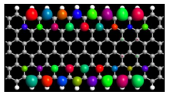
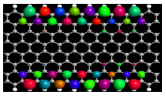
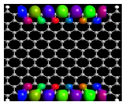
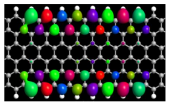
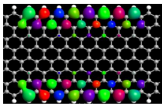
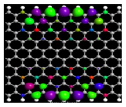
(a)

	1-ZGNR	2-ZGNR	3-ZGNR
Eigenstates and eigenvalues	 1.00	 1.00	 1.00
	 1.00	 1.00	 1.00
		 1.00	

(b)

	4-ZGNR	6-ZGNR	8-ZGNR
Eigenstates and eigenvalues	 1.00	 1.00	 1.00
	 0.97	 0.87	 0.86
	 0.96		
	 0.94		
	 0.89	 0.85	 0.84

(c)

	5-ZGNR	7-ZGNR	9-ZGNR
Eigenstates and eigenvalues	 0.98	 0.98	 1.00
	 0.94	 0.97	 1.00
	 0.83	 0.81	 0.98

SI-6 The transmission eigenstates and eigenvalues of (a) narrow ZGNR ($1 \leq n \leq 3$), (b) even ZGNR, and (c) odd ZGNR at zero bias.

SI-6 gives the eigenstates corresponding to the scattering state from the left

electrode to the right electrode. The transmission eigenvalue reflects the transmission probability of electrons from the left electrode to the right electrode. In **SI-6**, the eigenstates of the all ZGNRs are localized at the edge of the nanoribbon, and the transmission eigenvalues are almost close to 1.0, especially for the narrow ZGNRs. The interpretation of these results is that an electron incoming from the left electrode in the state with high transmission eigenvalue (close to unity) can easily transmit into the right electrode and hence it is declocalized over the junction.