Electronic Supplementary Information (ESI)

Graphene nanopores: electronic transport properties and design methodology

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SI 1. Transmission spectra of aGNPs

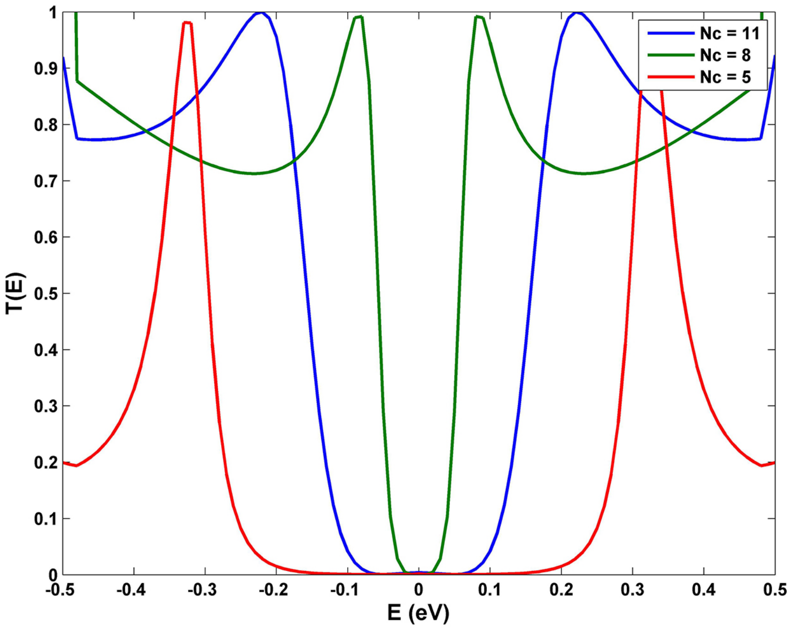

Figure S1 Transmission spectra of aGNPs with perfect (unbroken) pore edges created with a *Na=29* aGR. The pore length *Lc = 3* is fixed and pore width (*Na-2Nc*) is varying as *Nc* is altered. The change in the pore width leads to changes in the width of the "U"-shaped transmission spectrum around the Femi energy. The aGNP remains semi-conducting when pore width is changed.

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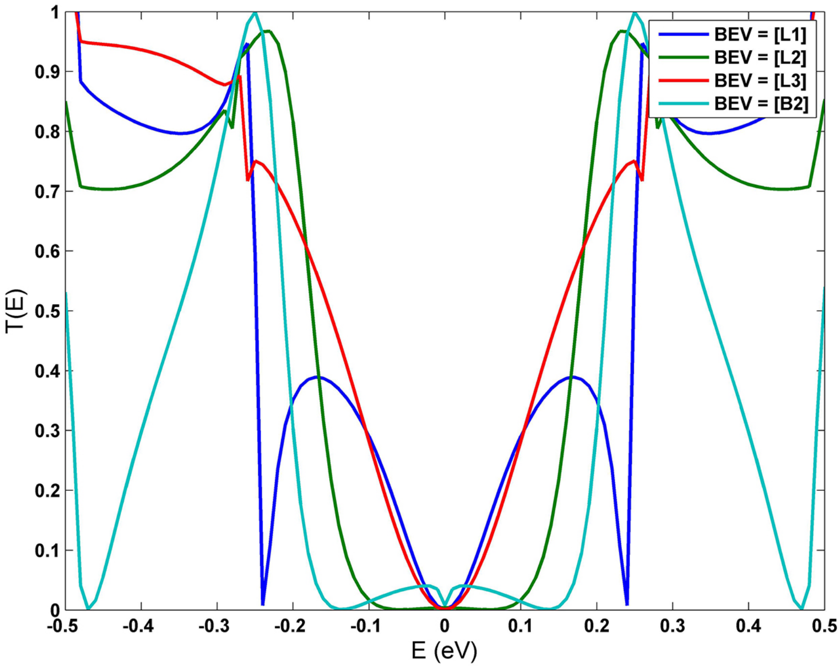

Figure S2 Transmission spectra of aGRs with one broken pore edge created with a *Na=29* aGR. The pore length *Lc* and width (*Na-2Nc=7*) are fixed by *Lc=3* and *Nc=11*. Removing a tip atom of the zigzag edge (*BEV = [L1]* or *BEV = [L3]*) leads to "V"-shaped transmission spectra. The aGNP remains semi-conducting when only one pore edge is broken.

SI 2. Transmission spectra and LDOS

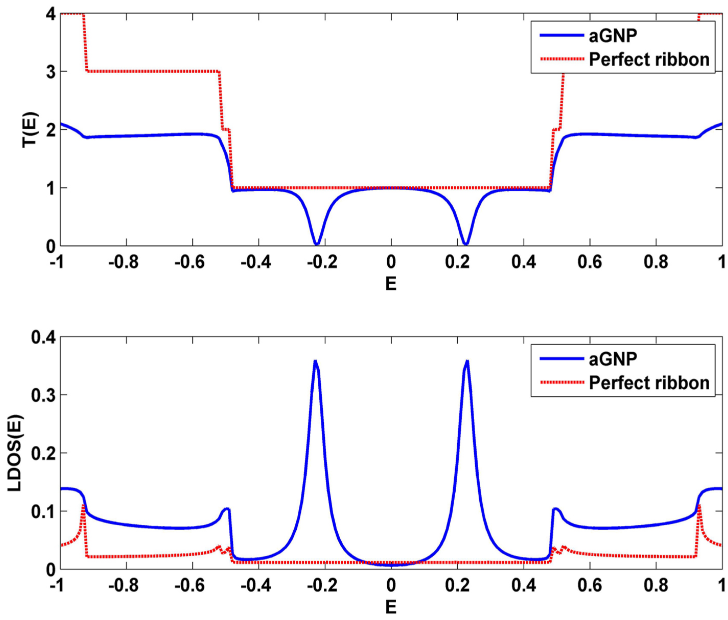

Figure S3 Transmission spectra and LDOS of perfect ribbon and aGNP in Fig. 2b with "∩"-shaped transmission (*i.e.*, with BEV=[L1, R5].) **a**, The transmission spectra. **b**, LDOS at the pore-edge atom located at L3. (See Fig.1 for pore geometries.)

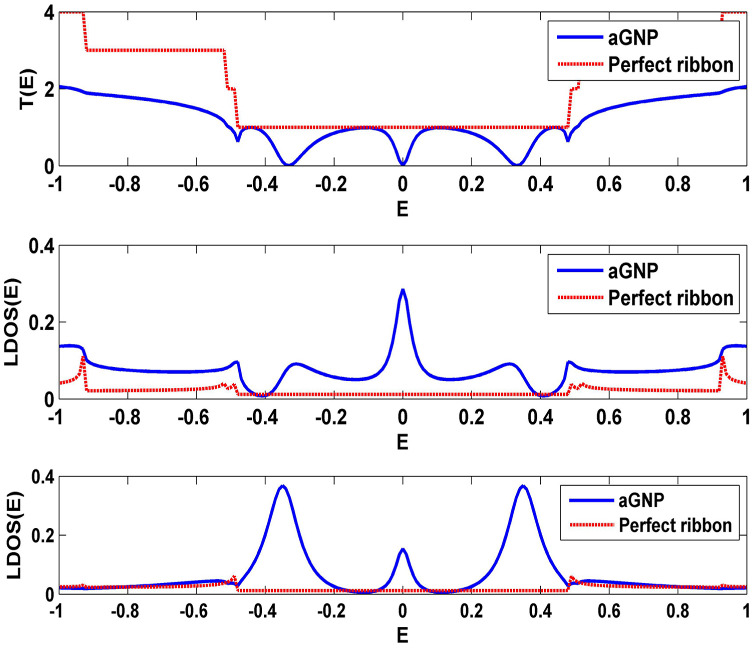

Figure S4 Transmission spectra and LDOS of perfect ribbon and the aGNP in Fig. 2b with "M"**-shaped transmission (i.e., with BEV=[L1, R3, T3].) a**, The transmission spectra. **b**, LDOS at the pore-edge atoms located at L3. **c**, LDOS at the pore-edge atoms located at T6. (See Fig.1 for pore geometries.)

SI 3. Derivation of transmission spectrum of the system shown in Fig. 3a

The QW has one conduction band with dispersion relation $E=2t_0cos(ka)$, where E is the energy of electrons, t_0 the hopping coefficient in the QW, k the wave number and a the lattice spacing. To calculate the transmission of this system, we assume that the electrons are described by a plane wave incident from the far left with unit amplitude and a reflection amplitude r. At the far right the wave has a transmission amplitude t. The probability amplitude to find the electron on site j of the QW in the state k can, therefore, be written as[1]:

$$a_j = e^{ikja} + re^{-ikja}, \quad j \le 0 \tag{1}$$

$$a_j = te^{ikja}, \quad j \ge L \tag{2}$$

where i is the imaginary unit. Solving the two equations obtained by setting $j=0$ and $j=-1$ respectively in (1) leads to

$$a_{-1} = -2i\sin(ka) + a_0 e^{ika}. \tag{3}$$

Similarly the equations of (2) on sites $j=L$ and $j=L+1$ leads to

$$a_{L+1} = a_L e^{ika}. \tag{4}$$

By defining $\tau = -E/t_0$, the Schrödinger equations on other sites of the QW are given by

$$-\tau a_j = a_{j-1} + a_{j+1}, \quad j = 1, \cdots, L-1. \tag{5}$$

Now consider the left QDC. The probability amplitude, b_l, to find the electron in the state l of the QDC obeys the following Schrödinger equations:

$$Eb_1 = \varepsilon_1 b_1 + V_1\, b_2 + t_1\, a_0, \tag{6}$$

$$Eb_l = \varepsilon_l b_l + V_1\, b_{l-1} + V_1\, b_{l+1}, \quad l = 2, \cdots, N_1 - 1, \tag{7}$$

$$Eb_{N_1} = \varepsilon_N b_{N_1} + V_1\, b_{N_1-1}. \tag{8}$$

Iterating backwards the equation for b_{N_1} we can express b_1 in terms of a_0:

$$b_1 = \frac{t_1\, a_0}{D_1}, \tag{9}$$

where

$$D_1 = Q_{N_1}(\varepsilon_1, V_1, N_1), \quad (10)$$

with Q_{N1} defined by

$$Q_1(\varepsilon, V, N) = E - \varepsilon, \quad (11)$$

$$Q_n(\varepsilon, V, N) = E - \varepsilon - \frac{V^2}{Q_{n-1}(\varepsilon, V, N)} \quad n = 2, \cdots, N. \quad (12)$$

Inserting (9) into the following Schrödinger equation on site *j=0* of the QW:

$$Ea_0 = t_0 a_{-1} + t_0 a_1 + t_1 b_1 \quad (13)$$

leads to

$$-\tau_1 a_0 = a_{-1} + a_1, \quad (14)$$

where $\tau_1 = -(E - \frac{t_1^2}{D_1}) / t_0$.

Similarly, working on the right QDC and site *j=L* of the QW, we have

$$-\tau_2 a_L = a_{L-1} + a_{L+1}, \quad (15)$$

where $\tau_2 = -(E - \frac{t_1^2}{D_2}) / t_0$ with $D_2 = Q_{N_2}(\varepsilon_2, V_2, N_2)$.

The system transmission spectrum $T(E) = |t|^2$ can then be computed by solving the set of *L+3* equations (3)-(5), (14) and (15) for the transmission amplitude *t* using Cramer's rule, with the result given by

$$t = \frac{-2i\sin(ka)}{e^{ikLa}\Delta},$$

where

$$\Delta = -(\tau_1 + e^{ika})(\tau_2 + e^{ika})\Delta_{L-1} + (\tau_1 + \tau_2 + 2e^{ika})\Delta_{L-2} - \Delta_{L-3},$$

with Δ_K being the $K \times K$ determinant

$$\Delta_K = \begin{vmatrix} \tau & 1 & 0 & \cdots & 0 \\ 1 & \tau & 1 & \cdots & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & \cdots & 1 & \tau & 1 \\ 0 & \cdots & 0 & 1 & \tau \end{vmatrix}.$$

References

1. Datta, S. *Quantum Transport: Atom to Transistor* (Cambridge University Press, Cambridge, 2005).