Edge currents in zigzag graphene nanoribbons and graphene-based topological insulator nanowires as a route toward high- ZT thermoelectrics

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The recent discovery of research on graphene—a single layer of graphite, an exact two-dimensional crystal —has drawn a lot attention due to its unique electronic structure and transport properties governed by the two-dimensional honeycomb lattice of carbon atoms. [1] The exploration of its thermal and thermoelectric properties has been initiated by measuring the thermopower and phonon thermal conductivity $K_{\rm ph}$ of graphene-based materials lately

Thermoelectrics transform temperature gradients into electric voltage and vice versa. Thus, careful tradeoffs are required to optimize the dimensionless figure of merit $ZT = \frac{S^2GT}{\kappa_{\rm el}+\kappa_{\rm ph}}$, which quantifies the maximum efficiency of a thermoelectric cycle conversion in the linear-response regime where small voltage $V = -S\Delta T$ exactly cancels the current induced by the small thermal bias ΔT. The devices with $ZT > 1$ are regarded as good thermoelectrics, but values of $ZT > 3$ are required for thermoelectric devices to compete in efficiency with conventional power generators and refrigerators.

Thus, a number of proposals have been put forth to evade the problem of high lattice thermal conductivity of large-area graphene that could open a pathway for its thermoelectric applications. Switching to quasi-one-dimensional graphene nanoribbons (GNRs) makes possible further enhancement of ZT where it has been predicted that long (~ 1 μm) GNRs with zigzag edges and disorder introduced along such edges could reach $ZT \simeq 4$ at room temperature. [3]

However, it is more advantageous to search for high-ZT devices among clean nanowires [2] since edge or surface disorder can affect electronic conductance significantly. In This work, we analyze electronic and phononic quantum transport through zigzag or chiral graphene nanoribbons (GNRs) perforated with an array of nanopores. Since local charge current profiles in these GNRs are peaked around their edges when Fermi energy is close to dirac point, drilling nanopores in their interior does not affect such edge charge currents but largely reducing heat transmission delivered by phonons in sufficiently long wires. The combination of these two effects can yield highly efficient thermoelectric devices with maximum $ZT \simeq 11$ at liquid nitrogen temperature and $ZT \simeq 4$ at room temperature achieved in ~ 1 μm long zigzag GNRs with nanopores of variable diameter and spacing between them. Our analysis is based on the π-orbital tight-binding Hamiltonian with up to third nearest-neighbor hopping for electronic subsystem, the empirical fourth-nearest-neighbor model for Dynamical matrix in phononic subsystem, and nonequilibrium Green function formalism to study quantum transport in both of these models.

The principal results in this work Fig. 3(a) shows that the largest $ZT \simeq 3$ at $T = 77$ K and $ZT \simeq 1.5$ at $T = 300$ K can be reached using (8,1)-CGNR. On the other hand, if the pore diameter takes a random value within some interval and the distance between the pores is varied, then we find a possibility to further optimize the figure of merit which can reach astonishingly large values, $ZT \simeq 11$ at $T = 77$ K and $ZT \simeq 4$ at $T = 300$ K, in the case of ZGNR-based device.

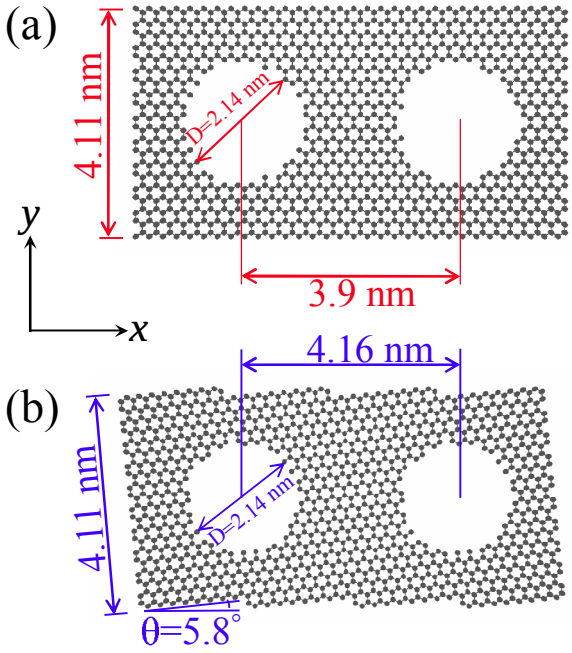

Fig. 1. (Color online) Schematic view of: (a) 20-ZGNR (composed of 20 zigzag chains); and (b) (8,1)-CGNR with chiral angle $\theta = 5.8^{\circ}$. The size of the nanopores, assumed to be drilled in the GNR interior away from its zigzag or chiral edges, and the distance between them is illustrated by plotting two repeated supercells of each GNR. The length of these GNRs in actual calculations is set to $L \simeq 1.2$ μm.

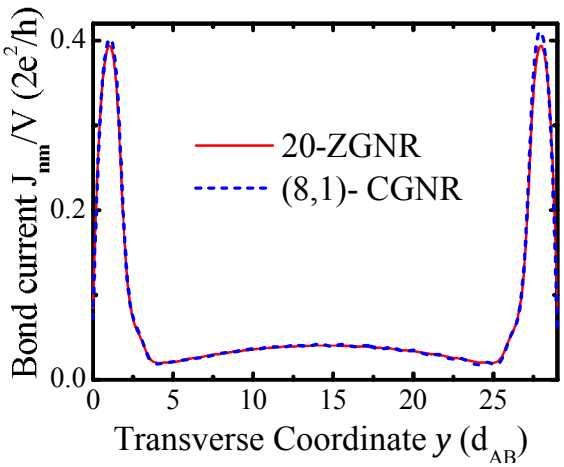

Fig. 2. (Color online) Spatial profile of local charge currents over the transverse cross section of infinite homogeneous 20-ZGNR or (8,1)-CGNR for electronic transport close ($E_F = -0.43$ eV) to the DP. The sum of bond currents [**?**] $J_{\mathbf{nm}}/V$, which describe charge flow from site $\mathbf{n}$ to site $\mathbf{m}$ of the honeycomb lattice if hopping $t_{\mathbf{n}}^{\mathbf{m}} \neq 0$ is non-zero between the two sites, gives the conductance $G = I/V$ (I is the total current in the leads and $V \to 0$ is small bias voltage driving the linear-response transport).

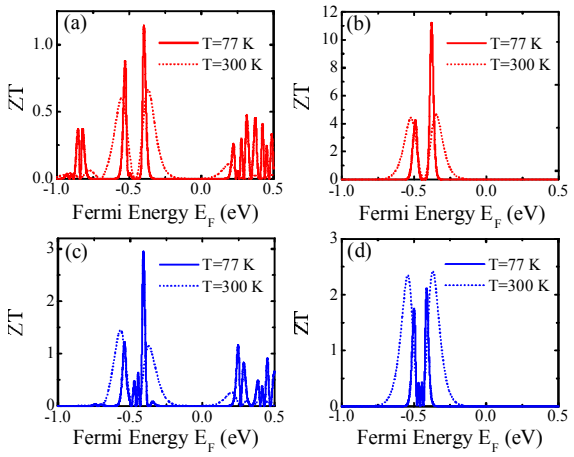

Fig. 3. (Color online) The thermoelectric figure of merit ZT for GNR+nanopores devices of length $L \simeq 1.2$ μm: (a) ZT vs. energy at two different temperatures for 20-ZGNR with a periodic array of identical nanopores illustrated in Fig. 1(a); (b) ZT vs. energy at two different temperatures for 20-ZGNR with pores of variable diameter $D \in [4.5\, d_{AB}, 7.5\, d_{AB}]$ and their position shifted by a value $\Delta x \in [-2\, d_{AB}, 2\, d_{AB}]$ along the transport direction away from the original position within periodic array shown in Fig. 1(a); (c) ZT vs. energy at two different temperatures for (8,1)-CGNR with a periodic array of identical nanopores illustrated in Fig. 1(b); and (d) ZT vs. energy at two different temperatures for (8,1)-CGNR with pores of variable diameter $D \in [1.5\, d_{AB}, 3.5\, d_{AB}]$ and their position shifted by a value $\Delta x \in [-0.5\, d_{AB}, 0.5\, d_{AB}]$ along the transport direction away from the original position within periodic array shown in Fig. 1(b).