Graphene nanopores for biosensing and thermoelectric applications: First-principles quantum transport simulation

Branislav K. Nikolić
Department of Physics & Astronomy, University of Delaware, Newark, DE 19716, USA
EMAIL: bnikolic@udel.edu | WWW: https://wiki.physics.udel.edu/qttg

Mechanical stability of graphene and advances in nanofabrication have recently made possible drilling of tiny holes (or arrays of such holes) of nanoscale diameter within graphene sheets. The experimental demonstration of DNA translocation through graphene nanopores has opened new avenues for third-generation DNA sequencing, where unlike traditionally considered biological or solid-state nanopores, one-atom-thickness of graphene means that only one nucleobase is present within the nanopore. However, the poor signal-to-noise ratio achieved in sensing of nucleobases within the nanopore via vertical ionic current calls for new ideas to exploit electronic transport in the plane of graphene. Using nonequilibrium Green function formalism combined with density functional theory (NEGF+DFT) simulations, we have predicted [1,2] that using edge currents in zigzag or chiral graphene nanoribbons (GNR) could significantly improve signal-to-noise ratio, thereby enabling ultrafast DNA sequencing.

An array of graphene nanopores can also be used to significantly impede the lattice thermal conduction through GNRs, decorated with heavy adatoms to locally enhance spin-orbit coupling and convert GNR into a two-dimensional topological insulator. The nanopores do not affect electronic current carried by helical edge states, which generate a highly optimized power factor per helical conducting channel due to narrow boxcar-function-shaped electronic transmission (surpassing even the so-called Mahan-Sofo limit obtained for delta function-shaped electronic transmission). In Ref. [3], we have predicted that thermoelectric figure of merit of GNR + heavy adatoms + nanopores system would reach its maximum $ZT \sim 3$ at low temperatures $T \sim 40$ K, which paves a way to design high-ZT materials by exploiting the nontrivial topology of electronic states through nanostructuring.

In this talk, I will overview these two classes of graphene nanopore devices, illustrated in Fig. 1, as well as challenges for NEGF+DFT simulations applied to their design and modeling.

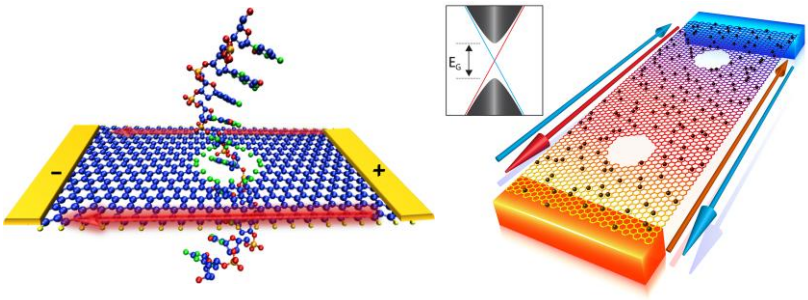

Figure 1: Schematic view of a single nanopore within GNR with zigzag or chiral edges for ultrafast DNA sequencing (left panel) [1,2]; or an array of nanopores within GNR (with arbitrary edges) and heavy adatoms for high-ZT thermoelectric applications by exploiting the nontrivial topology of electronic states (right panel) [3].

References

[1] K. K. Saha, M. Drndić, and B. K. Nikolić, Nano Lett. **12**, 50 (2012).
[2] P.-H. Chang, H. Liu, and B. K. Nikolić, J. Comput. Electron. **13**, 847 (2014).
[3] P.-H. Chang, M. S. Bahramy, N. Nagaosa, and B. K. Nikolić, Nano Lett. **14**, 3779 (2014).