GRAPHENE NANORIBBONS FAR FROM EQUILIBRIUM: FUNDAMENTALS, COMPUTATIONAL ALGORITHMS, AND NANOELECTRONICS APPLICATIONS

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The surprising discovery of graphene, as the first truly two-dimensional crystal where carbon atoms are arranged into a honeycomb lattice, has opened unforeseen avenues for basic research on transport and interactions in low-dimensional electron systems, bench-top testing of quantum electrodynamics, as well as for carbon nanoelectronics. While bulk graphene as a zero gap semiconductor is not suitable for digital electronics applications, the very recent fabrication of sub-10-nm-wide graphene nanoribbons (GNR) could make possible fabrication of complex nanoelectronic circuits from a single graphene sheet or molecular electronics with transparent contacts to conjugated molecules. This also requires substantial first principles quantum transport modeling to capture accurately electronic and atomistic structure of the devices and related charge transfer in equilibrium and charge redistribution under far-from-equilibrium conditions. In this talk, I will review recent advances in the so-called nonequilibrium Green function combined with the density functional theory (NEGF-DFT) approaches that we have utilized to explore: (i) GNR-based nanotransistors composed of thousands of carbon atoms; (ii) nonequilibrium phase transitions between magnetic insulating and non-magnetic metallic phases of GNRs with zigzag edges; (iii) how to employ the spin-dependent shot noise to detect magnetic ordering in GNRs with zigzag edges; and (iv) quantum interference effects in three-terminal GNR-molecule heterojunctions.

References

[1] http://web.physics.udel.edu/research/nanoscale-physics/graphene-nanoelectronics