Introduction

Branislav K. Nikolić

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The discovery of a wonder material *graphene*—the first one-atom-thick crystal whose honeycomb lattice of carbon atoms imposes gapless, massless and chiral Dirac spectrum on its low-energy quasiparticles—has swiftly ignited intense theoretical and computational studies of its unusual electronic transport properties. The “first wave” of such studies [whose results are summarized in, e.g., Rev. Mod. Phys. **83**, 407 (2011)] has been largely focused on explaining conductivity measurements at small bias voltage applied to large-area graphene samples as a function of carrier density, temperature and magnetic field, while typically relying on simplistic model Hamiltonians.

This Special Issue on *Electronic transport in graphene nanostructures and devices* contains a collection of sixteen papers which overviews what could be termed as the “second wave” of studies of electronic transport in graphene. Here the focus is on confined structures (such as nanoribbons and nanoflakes), graphene-based devices (such as transistors and *pn* junctions), and novel state variables (such as pseudospin in mono- and bi-layer graphene, real electronic spin, wavefunction phase, and properties of correlated many-body quantum states like exciton condensates).

The greatest roadblock to continued scaling of conventional silicon electronic for digital applications is the power dissipated in various leakage mechanisms. The quantum coherent transport regime and novel state variables in graphene offer a prospect for revolutionary device designs that go beyond traditional (silicon or carbon) field-effect transistors (FETs) based on classical physics [an overview of progress

in using graphene as a building block of conventional transistors can be found in Nature Nanotech. **5**, 487 (2010)]. For example, exploiting them would make possible to switch current off without utilizing energy barrier of traditional FETs, thereby evading thermal limitations in the subthreshold regime.

Concurrently, a number of papers in this special issue has covered the state-of-the-art computational algorithms for simulating quantum transport in graphene-based devices which can capture their atomistic structure (including input from first-principles calculations), possibly large number of carbon atoms in arbitrary measurement geometry, microscopic scattering mechanisms, and self-consistent charge transfer between different atomic species in equilibrium or charge redistribution when finite bias or gate voltage is applied. The coverage of specific algorithms is often very detailed, thereby allowing interested researchers and students to easily implement their own version.

The paper by Baraza-Lopez reviews application of non-equilibrium Green function combined with density functional theory (NEGF+DFT) approach to modeling transport through two-terminal metal/nanoscale graphene heterojunctions, while also introducing a procedure for obtaining tight-binding Hamiltonians that fit DFT-computed electronic dispersion at interfaces and whose combination with NEGF formalism can substantially speed up modeling of realistic devices. Wang, Guo, and Bevan show how NEGF+DFT formalism can be extended using nonequilibrium vertex correction to capture impurity scattering in a systematic fashion, which is then applied to compute the conductance of two-terminal graphene devices of nanoscale length and infinite width.

The effect of short-range potential scattering (due to point defects and/or dislocations) on the mobility of electrons in graphene on silicon dioxide, boron nitride and sili-

B.K. Nikolić (✉)
Department of Physics and Astronomy, University of Delaware,
Newark, DE 19716, USA
e-mail: bnikolic@udel.edu

con carbide substrates is analyzed in the paper by Ferry using semi-classical ensemble Monte Carlo approach. Cresti shows how to model chemical functionalization (such as with methyl-groups) of graphene nanoribbons (GNRs) using tight-binding Hamiltonian, which is then combined with NEGF formalism to study how electronic transport transitions from ballistic to diffusive and finally to localized (characterized by the opening of a transport gap) regime. The paper by Ramezani Masir and Peeters studies scattering of massless Dirac electrons in graphene by a random array of circular magnetic flux tubes.

A number of papers is devoted to discussing NEGF-based numerical techniques combined with tight-binding models of graphene. Sajjad, Polanco, and Ghosh show how to model graphene heterojunctions approaching experimental dimensions, including implementation of exact open boundary conditions along the edges to minimize spurious edge reflections, which is then applied to understand electron ‘optics’ and pseudospintronics in *pn* junctions made of monolayer graphene. The paper by Lewenkopf and Mucciolo offers comprehensive and pedagogical discussion of the recursive GF algorithms applied to the computation of conductance, density of states, and local current profiles in two-terminal graphene sheets and GNRs (including disorder, inhomogeneous gating, finite temperature, and even dephasing). Girão and Meunier review recently proposed “knitting and sewing” extensions of the recursive GF algorithms to multiterminal devices, while demonstrating how to combine them with parallel computing which paves the way to tackle systems composed of tens of thousands of atomic orbitals (example applications include graphene flakes attached to six GNR terminals). Liu provides a self-contained introduction to theoretical modeling of gate-induced carrier density in graphene sheets, including hands-on Matlab tutorials and applications to modeling of realistic experimental conditions for graphene *pnp* junctions and superlattices (thus obtained electrostatic potential is then easily introduced into electronic transport calculations based on NEGF formalism).

Nguyen *et al.* use numerical simulations, based on NEGF formalism combined with tight-binding models, to investigate different routes toward achieving strong negative differential resistance effect in graphene-based tunnel diodes and tunnel transistors, while also analyzing proposals for bandgap opening by nanostructuring graphene within such

devices. The paper by Souma, Ohmi, and Ogawa presents numerical simulations of the effect of various types of strain on gate-induced control of quantum transport in single layer graphene attached to two metallic electrodes.

The pseudospin represents the sublattice degree of freedom in the case of monolayer graphene, or the layer index in the bilayer (where two graphene monolayers are Bernal stacked to allow for interlayer hopping of electrons) and double-layer (where two graphene monolayers are separated by an insulating tunnel barrier) cases. The paper by Majidi and Zareyan reviews studies of pseudospin-polarized quantum transport in graphene-based heterostructures composed of normal regions, superconductors, and gapped regions acting as pseudoferrromagnets whose sublattice pseudospin symmetry-broken state has a net pseudomagnetization oriented perpendicularly to the plane of graphene. Bala Kumar and Guo study charge transport across pseudospin-valves made by combining monolayer, bilayer and hydrogenated-bilayer graphene to arrive at the conclusion that monolayer-bilayer junction might be an optimal choice for device applications. The paper by Dellabetta and Gilbert examines both equilibrium (using path-integral quantum Monte Carlo simulations) and nonequilibrium (using NEGF formalism) properties of superfluid phase in double-layer graphene due to indirectly bound excitons, including the effects of layer disorder and electron-phonon interaction.

The recent first-principles studies have suggested that low concentrations of suitably chosen heavy adatoms, even randomly deposited on graphene, could locally enhance the spin-orbit coupling (SOC) in graphene and convert it into the simplest realization of a two-dimensional (2D) topological insulator. This newly discovered phase of matter, which holds great potential for spintronic applications, is characterized by the bandgap in the bulk and chiral spin-polarized edge states which channel electrons of opposite spin to flow in opposite directions along the edges of the sample. Prada and Metalidis analyze quantum transport in heterostructures where GNR converted into 2D topological insulator is attached to a conventional metallic GNR, including the effects of edge disorder. The contribution by Carmier, Shevtsov, Groth, and Waintal studies the interplay of SOC and perpendicular magnetic or electric field on mono-, bi- and tri-layer graphene where the competition between quantum Hall and 2D topological insulator phases, as well as different types of the corresponding edge states, takes place.