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Cambridge University Press
978-1-107-03083-1 - Introduction to Graphene-Based Nanomaterials: From Electronic Structure to Quantum Transport
Luis E. F. Foa Torres, Stephan Roche and Jean-Christophe Charlier
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Introduction to Graphene-Based Nanomaterials

Beginning with an introduction to carbon-based nanomaterials, their electronic properties, and general concepts in quantum transport, this detailed primer describes the most effective theoretical and computational methods and tools for simulating the electronic structure and transport properties of graphene-based systems.

Transport concepts are clearly presented through simple models, enabling comparison with analytical treatments, and multiscale quantum transport methodologies are introduced and developed in a straightforward way, demonstrating a range of methods for tackling the modeling of defects and impurities in more complex graphene-based materials. The authors also discuss the practical applications of this revolutionary nanomaterial, contemporary challenges in theory and simulation, and long-term perspectives.

Containing numerous problems for solution, real-life examples of current research, and accompanied online by further exercises, solutions, and computational codes, this is the perfect introductory resource for graduate students and researchers in nanoscience and nanotechnology, condensed matter physics, materials science, and nanoelectronics.

Luis E. F. Foa Torres is a Researcher at the Argentine National Council for Science and Technology (CONICET) and an Adjoint Professor at the National University of Córdoba, Argentina, specializing in quantum transport with emphasis on inelastic effects and driven systems.

Stephan Roche is an ICREA Research Professor at the Catalan Institute of Nanoscience and Nanotechnology (ICN2), where he is Head of the Theoretical and Computational Nanoscience Group, focusing on quantum transport phenomena in materials such as graphene.

Jean-Christophe Charlier is a Professor of Physics at the University of Louvain, Belgium, whose interests include condensed matter physics and nanosciences. His main scientific expertise focuses on first-principles computer modeling for investigating carbon-based nanomaterials.

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Torres, Roche, and Charlier have written a very attractive book on graphene-based materials that takes a reader or student with no prior exposure to this topic to a level where he or she can carry out research at a high level and work in this area professionally, assuming a standard background of a condensed matter physics graduate student. The material is nicely organized into chapters which can be subdivided into daily learning segments and with problem sets that could be helpful for either formal course presentation or self study. Four appendices with more detailed presentations allow readers to develop the skills needed for using and extending present knowledge to advancing the science of few-layered materials or for developing applications based on these materials. All in all I would expect this to become a popular text for present and future researchers who will be active in the present decade, advancing science and launching technological innovation.

Mildred Dresselhaus, *Massachusetts Institute of Technology*

This book covers the fundamental aspects of graphene, starting from the very beginning. By reading this book, most basic subjects on graphene and some special theoretical methods can be understood at a high level. Starting with the current status of graphene science, the authors proceed to a self-contained description of the electronic structure of graphene, then an especially detailed description of the transport properties of graphene, such as back scattering, Klein tunnelling, quantum dots, Landau levels etc., based on the authors' work. Methods introduced to investigate these subjects range from the tight binding method to *ab initio* calculations, so that the readers can select their preferred method, and the appendices contain useful mathematical explanations for these methods. Thus, without reading the other textbooks, the reader can understand the text. The book should be useful not only for theoretical researchers but also for graduate students and experimental researchers, who will quickly understand the theorists' perspective. This book will be an important basic textbook on the physics of graphene.

R. Saito, *Tohoku University*

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From Electronic Structure to Quantum Transport

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Preface

Once deemed impossible to exist in nature, graphene, *the first truly two-dimensional nanomaterial ever discovered*, has rocketed to stardom since being first isolated in 2004 by Nobel Laureates Konstantin Novoselov and Andre K. Geim of the University of Manchester. Graphene is a single layer of carbon atoms arranged in a flat honeycomb lattice. Researchers in high energy physics, condensed matter physics, chemistry, biology, and engineering, together with funding agencies, and companies from diverse industrial sectors, have all been captivated by graphene and related carbon-based materials such as carbon nanotubes and graphene nanoribbons, owing to their fascinating physical properties, potential applications and market perspectives.

But what makes graphene so interesting? Basically, graphene has redefined the limits of what a material can do: it boasts record thermal conductivity and the highest current density at room temperature ever measured (a million times that of copper!); it is the strongest material known (a hundred times stronger than steel!) yet is highly mechanically flexible; it is the least permeable material known (not even helium atoms can pass through it!); the best transparent conductive film; the thinnest material known; and the list goes on ...

A sheet of graphene can be quickly obtained by exfoliating graphite (the material that the tip of your pencil is made of) using sticky tape. Graphene can readily be observed and characterized using standard laboratory methods, and can be mass-produced either by chemical vapor deposition (CVD) or by epitaxy on silicon carbide substrates. Driven by these intriguing properties, graphene research is blossoming at an unprecedented pace and marks the point of convergence of many fields. However, given this rapid development, there is a scarcity of tutorial material to explain the basics of graphene while describing the state-of-the-art in the field. Such materials are needed to consolidate the graphene research community and foster further progress.

The dearth of up-to-date textbooks on the electronic and transport properties of graphene is especially dramatic: the last major work of reference in this area, written by Riichiro Saito, Gene Dresselhaus, and Mildred Dresselhaus, was published in 1998. Seeking to answer the prayers of many colleagues, who have had to struggle in a nascent field characterized by a huge body of research papers but very little introductory material, we decided to write this book. It is the fruit of our collective research experience, dating from the early days of research on graphene and related materials, up through the past decade, when each of us developed different computational tools and

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theoretical approaches to understand the complex electronic and transport properties in realistic models of these materials.

We have written *Introduction to Graphene-Based Nanomaterials: From Electronic Structure to Quantum Transport* for everyone doing (or wishing to do) research on the electronic structure and transport properties of graphene-related systems. Assuming basic knowledge of solid state physics, this book offers a detailed introduction to some of the most useful methods for simulating these properties. Furthermore, we have made additional resources (computational codes, a forum, etc.) available to our readers at cambridge.org/foatorres, and at the book website (*introductiontographene.org*), where additional exercises as well as corrections to the book text (which will surely appear) will be posted.

Graphene and related materials pertain to a larger family that encompasses all kinds of two-dimensional materials, from boron nitride lattices, to transition-metal dichalcogenides (MoS_2, WS_2), to the silicon analogue of graphene, silicene, a recently discovered zero-gap semiconductor. Researchers are beginning to explore the third dimension by shuffling two-dimensional materials and by fabricating three-dimensional heterostructures (BN/graphene, BN/MoS_2/graphene, etc.) with unprecedented properties.

Interestingly, low-energy excitations in two-dimensional graphene (and in one-dimensional metallic carbon nanotubes), known as massless Dirac fermions, also develop at the surface of topological insulators (such as $BiSe_2$, Bi_2Te_3, etc.), which are bulk insulators. Topological insulators thus share commonalities with graphene, such as Berry's phase-driven quantum phenomena (Klein tunneling, weak antilocalization,. . .), and exhibit other features such as spin-momentum locking that offer different and ground-breaking perspectives for spintronics. Therefore, we believe that our presentation of the fundamentals of electronic and transport properties in graphene and related materials should prove useful to a growing community of scientists, as they touch on advanced concepts in condensed matter physics, materials science, and nanoscience and nanotechnology.

The book starts with an introduction to the electronic structures and basic concepts in transport in low-dimensional materials, and then proceeds to describe the specific transport phenomena unique to graphene-related materials. Transport concepts are then presented through simple disorder models, which in some cases enable comparison with analytical treatments. Additionally, the development of multiscale quantum transport methodologies (either within the Landauer–Büttiker or Kubo–Greenwood formalisms) is introduced in a straightforward way, showing the various options for tackling defects and impurities in graphene materials with more structural and chemical complexity: from combined *ab initio* with tight-binding models, to transport calculations fully based on first principles. To facilitate reading, the essential technical aspects concerning the formalism of Green functions, as well as transport implementation and order-N transport schemes are described in dedicated appendices.

This book encompasses years of scientific research that has enabled us to establish certain foundations in the field, a work made possible by the efforts of collaborators, including many postdoctoral and doctoral students. We are particularly indebted to Hakim Amara, Rémi Avriller, Blanca Biel, Andrés Botello-Méndez, Victoria Bracamonte, Hernán Calvo,

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We hope that you find this book to be a useful companion for starting in this field and perhaps even for your day-to-day research. We recommend that you start by reading Chapter 1 and then follow the advice in the *Guide to the book* (Section 1.3).

And we wish you an exciting journey in Flatland!. . .

Luis E. F. Foà Torres, Stephan Roche, and Jean-Christophe Charlier.

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