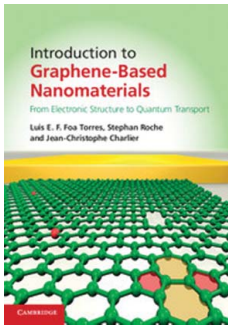
Acta Crystallographica Section B
Structural Science, Crystal Engineering and Materials
ISSN 2052-5206

book reviews

Works intended for this column should be sent direct to the Book-Review Editor, whose address appears in this issue. All reviews are also available from **Crystallography Journals Online**, supplemented where possible with direct links to the publisher's information.



Introduction to Graphene-Based Nanomaterials: From Electronic Structure to Quantum Transport. By Luis E. F. Foa Torres, Stephan Roche and Jean-Christophe Charlier. Cambridge University Press, 2014. Pp. 421. Price GBP 60.00, USD $ 98.00 ISBN 978-11078030831 (hardback).

Owing to the recent explosion of scientific activity around graphene and other two-dimensional materials, the number of textbooks and review articles on the topic has increased exponentially over the last few years. As far as I know, there is no recent book covering the particular aspects of transport in graphene, together with the pedagogical material needed to understand them. The book *Introduction to Graphene-Based Nanomaterials* with the subtitle *From Electronic Structure to Quantum Transport*, written by Luis E. F. Foa Torres, Stephan Roche and Jean-Christophe Charlier aims at filling this gap and offers to its readers a particular focus on the electronic and transport properties (as suggested by the subtitle) of graphene-based compounds, which is also a topic of the scientific research conducted by the three authors.

The book starts with a short preface, in which the authors address their motivation to write the book, together with the usual acknowledgements to their co-workers in the field. This is followed by the first chapter of the book, entitled 'Introduction to carbon-based nanostructures', which reminds the reader about the basics of carbon chemistry (hybrid orbitals) and presents some of the various carbon nanostructures, mainly from a historical point of view. The chapter is closed by a guide to the book which describes shortly each part of the book, and a 'further reading' section which contains references related to this introductory chapter.

The second chapter ('Electronic properties of carbon-based nanostructures') starts by introducing the electronic structure of graphene *via* tight-binding models. Although this is well known to the experienced readers, beginners in the field will certainly take here the opportunity to derive these models on their own and compare them with those presented in the book, which is crucial to understanding the notions of Dirac cones, trigonal warping and the other particularities of the electronic structure of graphene. A difficulty concerns the paragraph on 'phase ambiguity and Berry phase', which is probably not straightforward to understand for a beginner and might require further reading outside the book to become understandable. Starting from p. 23, the tight-binding band structures are compared with those obtained from more advanced theories, therefore, at this point a beginner will probably feel the need to read Appendices A and B on *ab initio* calculations, while an experienced reader can safely continue his/her journey through the book.

The next section presents the electronic properties of few-layer graphene again by the means of a tight-binding model, followed by a short description of the corresponding *ab initio* results. This section could have been extended by introducing the electronic structure of rotated graphene layers (which are, however, mentioned in a footnote) and a short description of the van der Waals interactions that bind graphene layers together. The two next sections about graphene nanoribbons and carbon nanotubes contain the expected text and references needed to understand their respective electronic structures and how they are linked to that of graphene. §2.6 is quite short (two pages), but probably sufficient to capture the effect of spin-orbit coupling in graphene. The next section covers the effect of a magnetic field on the electronic structure of graphene-related materials, in particular the appearance of Landau levels and the Aharonov–Bohm effect. This section will require some extra attention from the readers to be understood, but the effort is worth doing when knowing the importance of the phenomena described. The last section of chapter 2 nicely presents the various defects that can occur in graphene, at graphene edges, and in carbon nanotubes. The notion of point defects (Stone–Wales and other reconstructions) and extended defects are presented *via* some very clear schematic representations together with some detailed explanations. The chapter is closed by some suggestions for further reading and a set of 12 problems, mostly about tight-binding Hamiltonians. Interestingly, one of the problems provides the necessary input files for the reader to run the *ABINIT* code (a freely available electronic structure package) in order to obtain the band-structure of graphene using density functional theory, which is certainly a good initiation to *ab initio* methods.

With the third chapter begins the second part of the book, focusing on transport properties. In this chapter of 25 pages, some general concepts are introduced followed by a discussion on coherent and decoherent transports. Landauer–Büttiker theory is introduced and the Kubo conductivity formula is derived in detail, and some illustrations in the cases of ballistic and diffusive regimes are provided. Importantly, a subsection entitled 'Kubo versus Landauer' aims at explaining which theory is applicable in what context. The chapter is concluded with three problems concerning electronic transport. Notice that here appendices C and D concerning the algorithmic of transport calculations can be read in parallel to this chapter.

The fourth chapter starts by presenting Klein tunnelling, and by using Hamiltonians relevant for low-energy physics (in connection with the equations derived in chapter 2), the difference between the transmission probabilities for a graphene monolayer and a graphene bilayer is demonstrated explicitly. In the second part of this chapter, ballistic transport in several carbon-based materials is discussed, and the nearest-

neighbour Hamiltonian of a zigzag carbon nanotube is derived in detail. Then Fabry–Pérot conductance oscillations are presented, followed by a paragraph on the important problem of contact effects with detailed discussions on several systems, for instance junctions made of metal/semiconducting nanotube/metal. This chapter ends with the usual 'Further reading' section, and seven problems on the topics introduced previously. The only slight criticism concerning this chapter is the fact that it is not always obvious to see the link between the two parts of the chapter: the similarity between Klein tunnelling and ballistic regime is mentioned in the last section, but could have been mentioned earlier in the chapter.

The next chapter is entitled 'Quantum transport in disordered graphene-based materials'. The description of effects related to disorder is essential since it brings theory closer to the true experimental situation. The chapter starts with a rather complete discussion on the concept of elastic mean free path, followed by a remarkable discussion on the transport properties of graphene. The Anderson model for disorder is introduced, and the regimes of weak and strong localization are presented. Then, possible sources of disorder in graphene are presented, such as monovacancies or the existence of various (polycrystalline and amorphous) forms of graphene, and the effect on mean free paths and localization lengths is discussed. The chapter is ended by five problems to be solved.

The sixth chapter introduces quantum transport beyond direct current (DC), which is relevant in alternating voltages or under light illumination. The chapter is quite short but well written and precise: Floquet theory to take into account a time-periodic potential in the Hamiltonian is presented and the equations for the average current and density-of-states are derived. Then, the effect of a laser on the electronic structure of graphene is presented. Since most of the cited references are quite recent, the reader will certainly enjoy reading the recommended supplementary reading. As usual, the chapter closes with a set of exercises, in this case three.

Chapter 7 is devoted to transport in graphene-based materials with impurities or disorder. After an introductory section, the electronic structure and transport properties of boron-doped or nitrogen-doped nanotubes are presented using a modified tight-binding Hamiltonian. In particular, the effect of a random distribution of N atoms on the conductance is presented in detail.

The next section presents some recent studies showing the impact of oxygen and hydrogen adatoms on the transport properties of graphene. However, this part could have been more detailed concerning the use of the Hubbard model in this particular framework. The following section (§7.4) is strongly linked with §2.8 since it concerns the effect of point defects in graphene. §7.5 is a long text continuing on the properties of nanotubes but also presenting recent works on graphene nanoribbons. It explains in detail the effect of the defects and of the doping on the conductance of nanotubes. Then the functionalization of nanotubes is introduced, with some particular examples treated with care like nanotubes with metal clusters. The second part of this section covers the properties of graphene nanoribbons. A quite complete overview is given concerning their various geometries and electronic structure properties taking into account point defects, edge disorder or doping. Finally, arrays and networks of graphene nanoribbons together with their conductance properties are shown.

The eighth and last chapter, entitled 'Applications', aims at presenting some promising applications of graphene. The chapter is surprisingly short considering all the efforts of the scientific community towards making use of graphene in applied science. However, it contains the expected material about the possibility of using graphene in electronics (including spintronics), for information storage, or together with light irradiation.

The main body of the book is then followed by four appendices. Appendix A presents briefly some well known methods used in solid-state physics for electronic structure calculations, namely the Hartree and Hartree–Fock approximations, and of course density functional theory. This methodological part is followed by a more practical part introducing pseudopotentials and plane waves. Appendix B is quite short and focuses on the *GW* approximation and its implementation as a perturbation over density functional theory. Appendix C is devoted to the Landauer–Büttiker formalism. The decomposition of the problem in a local basis is presented together with the necessary Green's functions algebra. Then, the computation of transport properties by *ab initio* calculations is developed, and a list of codes performing it is given. Albeit the topic might be difficult for a beginner, the text is pedagogical enough to be understandable. Finally, the last appendix presents in a few pages the Lanczos algorithm and the wave-packet propagation method. Last but not least, the book has a companion website (http://www.introductiontographene.org) with hints and solutions to some problems presented in the book, a collection of additional problems to solve, a list of links to available resources related to graphene, and the possibility to subscribe to a newsletter in order to be informed of the latest additions to the website. According to the book's preface, a forum and possible corrections to the text will also appear there. This is a quite innovative way to proceed and certainly adds even more value to this book. Of course, there is no such thing as a perfect book, and the only real criticism that I have concerns the lack of a (even short) chapter concerning graphene cousins such as, for example, monolayers of transition metal dichalcogenides and hexagonal boron nitride: these materials are briefly mentioned in the preface, but nothing more. Although the title clearly states that the book is about graphene-based materials, these even newer materials could have fit nicely in a chapter entitled 'Perspectives'. The authors may perhaps consider the possibility of writing a second book covering the properties of two-dimensional materials not based on graphene, but before that I can only recommend to students and researchers interested in graphene to buy, read and study the book written by Foa Torres, Roche and Charlier.

Sébastien Lebègue

Faculté des Sciences et Technologies, Université de Lorraine, Institut Jean Barriol FR 2843, CRM2 UMR-CNRS 7036, BP 70239, F-54506 Vandoeuvre-lès-Nancy CEDEX, France