

# Preface

The trend in the miniaturization of electronic devices has naturally led to the question of whether or not it is possible to use single molecules as active elements in nanocircuits for a variety of applications. The recent developments in nanofabrication techniques have made possible the old dream of contacting individual molecules and exploring their electronic transport properties. Moreover, it has been shown that molecules can indeed mimic the behavior of some of today's microelectronic components, and even strategies to interconnect molecular devices have already been developed. These achievements have given rise to what is nowadays known as *Molecular Electronics*. There are still many problems and challenges to be faced to make this novel electronics a viable technology, but the exploration of molecular-scale circuits has already led to the discovery of many fundamental effects. In this sense, molecular electronics has become a new interdisciplinary field of science, in which knowledge from traditional disciplines like physics, chemistry, engineering and biology is combined to understand the electrical and thermal conduction at the molecular scale.

This book provides a comprehensive overview of the rapidly developing field of molecular electronics. It focuses on our present understanding of the electrical conduction in single-molecule circuits and presents a thorough introduction to the experimental techniques and the theoretical concepts. To be precise, our goal in this monograph is two-fold. On the one hand, we want to provide a true textbook for advanced undergraduate and graduate students both in physics and chemistry who are interested in the field of molecular electronics or nanoelectronics in general. Our idea is to take a student with a good background in quantum mechanics all the way to be able to follow the specialized literature in molecular electronics or to start working in this field. On the other hand, we also want provide a

thorough review of the recent activities in molecular electronics from which newcomers and specialists in the field can benefit.

Bearing these goals in mind, this book has been written in a self-contained and unified way. It contains four parts that can be read independently. In the first two ones we review the basic experimental techniques and the main theoretical concepts concerning the electronic transport in atomic-scale junctions. These two parts are meant to be textbook material for an advanced course in molecular electronics. In particular, we have included a collection of exercises at the end of most chapters, which in many cases are motivated by recent experiments in the field. On the other hand, Part 3 contains two chapters in which we describe at an introductory level the physics of metallic atomic-size contacts and we also point out some of the remaining challenges and open problems in this context. Finally, Part 4 is devoted to the electrical and thermal transport in molecular circuits, with special emphasis on single-molecule junctions. Here, we do not only review the recent activities in the field of molecular electronics, but we also introduce the addressed topics at a basic level. In this sense, we have often included unpublished material and additional exercises to help the reader to gain a deeper insight into the fundamental concepts involved in the field of molecular electronics.<sup>1</sup>

We have tried to cover in this monograph as many aspects of molecular electronics as possible, but obviously the selection is limited for space reasons and it reflects unavoidably our own research interests. We also want to apologize with those authors that feel that their contribution was not properly highlighted in the review part of this monograph, but it is by now impossible to include all the huge amount of work done in this field. Finally, we just hope to have achieved, at least partially, the goal that truly motivated the writing of this book, namely the sincere will to provide a useful book for the new generation of researchers that should consolidate molecular electronics as a solid pillar of the emerging nanoscience.

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<sup>1</sup>See section 1.3 for a more detailed description of the structure and scope of the book.