

PREFACE

The understanding of the microscopic processes occurring in solids and liquids is a significant challenge for computational physics. The rapid growth of computer power including the new parallel architectures has stimulated a ferment of new theoretical and computational ideas which make now feasible to solve the basic physical equations for models of realistic complexity and to start to develop ab-initio material science, where the full complexity of real materials is taken into account together with a description of the microscopic interactions from first principles. We can say that more computer power means more physics because more realistic models can be studied and better theories can be used. The richness of the physics of condensed matter systems makes for computational physics to meet this challenge very rewarding.

Complexity occurs at different levels: on one side one wants to describe systems which are not reducible to few atoms periodically arranged: low dimensional solid systems (surfaces, interfaces, clusters), semiconductor devices, or disordered matter like liquids and random alloys. On the other side we have systems characterized by complex many-body correlations like quantum fluids or systems where there is a strong interplay between the ionic motions and the electronic degrees of freedom like in a liquid semiconductor. Finally complexity can also mean the study of phase transitions and of non-equilibrium properties such as thermodynamic processes and chemical reactions where multiple time and length scales are typically present.

The aim of this book is to describe some of the recent advances in the computer simulation of condensed matter systems, including quantum mechanics of many-particle systems, electronic properties, stability and phase transitions in complex materials, transport properties in realistic electronic devices, thermodynamic processes and chemical reactions. The methods used range from ab-initio (Car-Parrinello) molecular dynamics to quantum Monte Carlo simulations, self-consistent density functional approaches and to classical molecular dynamics simulations.

A number of advances in the theoretical approaches and in the algorithms are reported together with some examples of significant applications. We like to mention the extension of ab-initio molecular dynamics to a fluctuating simulation cell (Chapter 1), thus unabling the study of structural phase transitions in a more fundamental way than it was possible before, the development of a wave function that for the first time is able to describe a self-bound quantum fluid or a solid via interparticle correlations only (Chapter 2), advances in the simulation of rare events with application to some simple models of a chemical reaction (Chapter 5), the implementation of KKR-CPA method to study electronic topological transitions (Chapter 6) and of the LMTO code for ab-initio investigations of surface electronic properties (Chapter 7), and a

novel simulative approach to describe transport properties in semiconductor devices (Chapter 4). Some contributions are more exploratory in character and introduce some new ideas on how to solve some open problems such as the solution of the sign problem in a Fermion simulation (Chapter 3), at least at the level of a specific trial function.

An effort has been made to present not only the physical aspects and some typical results of these studies but, where appropriate, to discuss in some details technical aspects of the algorithms and computer codes that have been developed by the authors. Often these aspects are not very much discussed in the literature but they can be of great help to newcomers in the field.

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