

Preface

The 1st International Symposium on Computational Sciences (ISCS2011) took place from April 18 to April 21, 2011 in Shanghai, China. The scientific program of this symposium included many topics related to the methodological development and application of quantum simulations in biology and in the material sciences. The program consisted of plenary and regular presentations and included the following four main themes:

- Recent development of quantum mechanical methods,
- Simulations of biological systems,
- New techniques in material sciences, and
- New techniques in drug design and discovery.

In addition, a workshop on the theory, code and application of DFTB+ method was held on April 21, 2011.

This volume comprises ten chapters written by the selected presenters. These contributions cover three challenging areas in the field of computational sciences: (i) the development and utilization of quantum mechanical methods for improving the accuracy of the system, (ii) the application of computational simulation techniques for investigating the time-scale involved in the processes, and (iii) the generation of more rigorous molecular force fields to solve the problems of systems with significantly large sizes. This book aims to assemble overviews of recent developments as well as some applications of all these three computational techniques. Main focuses of this volume are the methodology and applications of the density functional theory (DFT) method in material sciences and the principles and applications of the combined quantum mechanical molecular mechanical (QM/MM) approach for the biological systems.

One of the key components in DFT theory is the exchange-correlation functionals. Their application in material sciences was reviewed and analyzed by Professor Pietro Cortona in the first chapter. On the other hand, the time-dependent (TD) approach was generally used to calculate the electronic excitations within the DFT frame. In Chap. 2, Professor Thomas Niehaus presents the implementation of the TD algorithm into DFTB+ method to simulate the quantum transportation process

between the metal leads. For the application of the DFT method in large systems such as nanoparticles, Professor Rui-Qin Zhang *et al.* (Chap. 3) used the DFTB+ method to investigate the optical properties of Silicon quantum dots (SQDs) for biological probes and sensors, and Professor Stephan Irle *et al.* described some important QM/MM simulations on the nucleation process of the carbon nanotubes in Chap. 4. In Chap. 5, Professor Zhenyu Li presented how to determine structures and properties of new material such as graphene oxide from a theoretical perspective.

The biological section was firstly highlighted in Chap. 6 by Professor Jeffrey Reimers who describes the recent development on the refinement of X-ray structures of biological system using DFT method. It is followed by Professor Thomas Simonson who in Chap. 7 outlined the current methods available for protein design and engineering and presented a recent application of his design technique for an important family of enzymes. It evokes some possibility of quantum mechanical methods for protein engineering and drug design. The later was discussed by Professor Ying Xue who in Chap. 8 presented their recent works on the ligand-based design of inhibitors of factor Xa using supported vector machine (SVP) method. The DFT method, in the frame of combined QM/MM methodology, has been widely used to quantitatively understand the mechanism of biological processes. In Chap. 9 Professor Dingguo Xu has reviewed some principles and applications of the QM/MM method for the enzyme catalytic mechanism of several biological systems. Finally in Chap. 10, Professor Bo Durbecj brought the application of this method to the excited states by presenting some recent studies in the photochemistry of phytochromes.

We hope that this consolidated volume will give its readers some insights into the recent progresses made in the field of quantum simulations for material and biological systems.

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