

PREFACE

There is no doubt that many of the readers of this book series wonder how the research/computational facilities will look like in the near future. It seems that the efficiency and compactness of the silicon-based computers are almost exhausted, and for significant progress one has to look for alternative solutions. A very promising future for computing is based on molecular computers. Among the molecular elements required for such computers, the developments rely on the existence of nanostorage devices.

A recent *Science* article (Z. M. Liu, A. A. Yasseri, J. S. Lindsey, and D. F. Bocian; *Science*, **302**, 1543, 2003) reveals silicon-tethered porphyrins that are resistant to heat (up to 400°C) and harsh conditions. Since porphyrins possess well known data storage characteristics, the unique properties of these new derivatives reveal the possibility for their commercial production. It is assumed that porphyrin-based memory chips can be assembled using facilities devoted to the traditional silicon devices, opening the way toward nano components of molecular computers.

The research in this area is extensive. To assist the readers, we have decided to collect more chapters for this book that are devoted to the reviews of current advances in nano science. As a result, this volume includes three chapters related to this important research area.

The first chapter, written by J. J. Palacios, A. J. Pérez-Jiménez, E. Louis, E. San Fabián, J. A. Vergés, and Y. García, reviews fundamental issues underlying first-principle quantum theory in atomic and molecular systems. The authors have recently developed a new approach called Gaussian Embedded Cluster Method that is based on the GAUSSIAN98 and GAUSSIAN03 codes. The review provides numerous examples that illustrate the applicability and reliability of this method. This is supported by the study and interpretation of various experiments in the field of molecular electronics.

Apparently, an ultimate goal of nano sciences is the development of tools for spatial and chemical control of single molecules. Among the experimental techniques that have emerged in recent years are single molecule fluorescence, optical and magnetic tweezers, and atomic force spectroscopy. All of these techniques allow for mechanical manipulations of single molecules. The proper comprehension of the experimental results requires adequate theory. W. Nowak and P. E. Marszałek present an overview of

recent advances and trends in the applications of computer simulations aimed at understanding atomic force microscopic experiments. Those variants of classical molecular dynamics (MD) simulations which are particularly helpful in the interpretation of experimental data obtained for single biopolymer molecules, such as steered MD or biased MD, are reviewed and discussed in detail.

In the third chapter, J. Seminario, P. Derosa, L. Cordova, and B. Bozard discuss the application of combined molecular dynamic simulations based on *ab initio* force fields and signal processing techniques to analyze the dynamic properties of nanocells. The analysis includes several characteristic modes at different temperatures. The authors consider the applications of such techniques for the characterization of new, molecular electronics.

The prediction of the excited state properties of molecular systems are among the most challenging tasks of computational chemistry. They are assisted by the development of new methods designed for such tasks. The most accurate approaches are based on the coupled cluster theory. D. Mukherjee and his group (S. Chattopadhyay, D. Pahari, and U. S. Mahapatra) review formulations of linear response theory for excited state potential energy surfaces which are based on multi-reference coupled electron-pair approximation categories of methods. This review includes a thorough discussion of the genesis of the developed theory. In addition, applications to the potential energy surfaces of low-lying excited states of the model P_4 and Li_2 molecules are also provided.

Recently progress has been achieved in the theoretical prediction of the magnetic exchange coupling constants in compounds of rare earth transition metals. In the fifth chapter, M. Atanasov, C. Daul, and H. U. Güdel describe a method developed for such tasks. After a comprehensive discussion of the calculation procedure, the authors present examples of its application to various dimers of rare earth metals.

My recent web search of the phrase “hydrogen bonding” resulted in over 50,000 entries. This demonstrates the popularity of this topic which was formally recognized more than 80 years ago. Over the years new and intriguing aspects of this phenomenon have been studied. Such studies reveal new classes of hydrogen bonds. One of such new categories, dihydrogen bonds (DHB), are discussed in the last chapter of this volume. S. J. Grabowski and J. Leszczynski present the examples of such interactions existing in crystal structures. These interactions are compared with the conventional hydrogen bonds. A comparison shows that DHBs are often similar to typical H-bonds. The discussion includes the results of *ab initio* calculations,

decomposition energy, topological parameters, and experimental neutron diffraction results.

I would like to thank all authors for the excellent contributions and fine collaborations. The very efficient technical assistance of Dr. Manoj K. Shukla in putting together this volume is greatly appreciated. As always, your feedback is very important to me, please feel free to e-mail your suggestions to jerzy@ccmsi.us.

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