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PREFACE

Intermolecular interactions constitute one of the major forces determining numerous specific properties and self organization of condensed matter including biological systems. There is no better illustration of their importance than the introduction in the famous textbook *The Feynman Lectures on Physics*:

If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis that all things are made of atoms – little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.

This statement refers directly to the concept of the potential energy function describing interaction energy as a function of the distance sufficient to model various properties of matter that are directly or indirectly related to the intermolecular forces. Recent progress in computational and experimental techniques opens the perspective for rational *de novo* design of new materials with desired properties being governed by specific interactions.

The main purpose of this volume is to present an overview of selected state-of-the-art computational methodologies and to present examples of applications. The first six chapters contain an in-depth description of several new techniques applied in modeling and designing new molecular materials.

The first chapter by Moszyński presents in a systematic and comprehensive manner the current state-of-the-art theory of intermolecular interactions. Numerous examples illustrate how theoreticians and experimentalists working in tandem may gather valuable quantitative results related to intermolecular interactions, like accurate potential functions, interaction-induced properties, spectra and collisional characteristics or dielectric, refractive or thermodynamic properties of bulk phases. On the other hand the most advanced Symmetry Adapted Perturbation Theory (SAPT) enables validation of more approximate variation-perturbation models which could be applied to the analysis of specific interactions in much larger molecular systems, for example enzyme-drug interactions discussed in Chapter VIII by Berlicki *et al.*

The second chapter by Wesołowski presents a general overview of the recent developments in Density Functional Theory (DFT), which currently constitutes the most popular tool for modeling molecular materials. Particular emphasis has been

given to the systematic discussion of approximations employed in DFT and their performance for various types of molecular aggregates.

Mezoscopic and microscopic modeling methods applied in modeling biopolymers are reviewed in the third chapter by Lesyng and coworkers, allowing for a better description of biomolecular recognition processes as well as corresponding free energy changes.

The fourth chapter by Michalak and Ziegler presents an excellent introduction into DFT-based first principle molecular dynamics capable of modeling complex chemical reactions. Considerable effort has been made by the authors to explain in detail the specifics of *ab initio* calculations wherever they differ from conventional techniques.

A very promising methodology bridging quantum mechanics and molecular mechanics (QM/MM), allowing the mechanisms of enzymatic reactions to be analyzed in detail, has been reviewed in the fifth chapter by Mulholland and Grant.

The chapter written by Ramos and coworkers reviews various computational techniques used to study protein-protein interactions, with particular attention given to thermodynamic characteristics of mutated proteins and their interactions.

The contribution of Paneth and coworkers demonstrates how substrate-enzyme interactions could be explored using experimentally determined kinetic isotope effects and QM/MM calculations.

The remaining three chapters illustrate various applications of molecular modeling methods in exploring various properties of complex protein systems. Nakano and coworkers analyse the mechanism of [NiFe] hydrogenase involved in hydrogen production. Renugopalakrishnan studies bacteriorhodopsin which is important in information storage technologies. Filipek and coworkers concentrate on rhodopsin as being an important target for pharmacological intervention.

Intermolecular interactions define crucial characteristics of materials for hydrogen storage materials. This topic is discussed in detail in the chapter by Cheng *et al.* devoted to molecular dynamics simulations of single-walled carbon nanotubes (SWNT) with molecular hydrogen. The properties of modified SWNTs, in the contribution from Politzer *et al.*, are also analyzed from the point of view of potential applications in molecular electronics.

Molecular electronic applications are also covered in the contribution from Zhou and Hagelberg discussing interactions of various organic molecules with silicon surface, whereas Zhou *et al.* concentrate on fullerene deposition on silicon and GaAs surfaces.

The last chapter by Michalkova *et al.* presents a review of the experimental and theoretical data on nerve agent interactions with different surfaces. Particular attention is given to molecular simulations of interaction and decomposition of phosphoroorganic compounds on various metal and metal oxide clusters.

Of course the examples discussed in this volume cover only a small fraction of possible applications. We hope that with the rapid progress of computational techniques many more molecular materials will soon be the subject of rational design *in silico*.

Let me express my gratitude to all authors for their contributions which will guide readers into the exciting world of molecular modeling.

W. Andrzej Sokalski
Wrocław, Poland
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