

Preface

The extraordinary developments of scientific computers during the past 50 years, together with the advances of theoretical chemistry have made possible, for the time being, the computations with great accuracy of the properties of molecular systems comprising about a hundred atoms. However, many systems of chemical or biochemical interest are much larger than allowed by the present limits of computational chemistry. For example, the apparently simple system made of a molecule dissolved in a solvent may exhibit properties quite different from those observed or computed in the isolated state. Similarly, the properties at the interface of a liquid, or a solid and a gas are expected to be quite different from those predicted for a not interacting molecule. The case of biochemical systems is a very typical example since a large number of systems of interest are made of thousands of atoms and if, from a chemical point of view, one feels allowed to focus on the chemical or physical part of interest, the interactions with the rest of the system cannot be discarded.

Historically, accounting for the solvent effects in quantum chemical computations became possible, in a rather simplified representation of the solvent by a dielectric continuum, more than 40 years ago.¹ In the meantime, the development of classical force fields opened the way to molecular mechanics i.e. the classical computation of intermolecular interaction energies and consequently the prediction of thermodynamic properties of these systems, thanks to statistical mechanical tools.

Finally, the coupling of an elaborated quantum description of a chemically important subsystem with the rest of the system described at a lower level such as the classical mechanical one or even the continuum allowed the development of multiscale models for the treatment of the complex systems considered above. These methodologies represent a real scientific advance which has been recently acknowledged by the Nobel prize awarded to Martin Karplus, Michael Levitt, and Arieh Warshel.

¹D Rinaldi and J-L Rivail, Polarisabilités moléculaires et effet diélectrique de milieu à l'état liquide. Etude théorique de la molécule d'eau et de ses dimères. *Theor. Chim. Acta*, 1973, **32**, 57–70.

The present book aims to cover various aspects of the state-of-the-art of computational treatment of complex molecular systems. This includes the development of accurate force fields, including induced electronic polarization and the applications of lower level models, in particular hybrid Quantum Mechanical/Molecular Mechanical (QM/MM) approaches to various problems such as solutions in which the solute–solvent and solvent–solvent interactions can be quite important, in particular in the case of aqueous solutions. The case of molecules at water–air or water–organic liquid interfaces is a special example of the necessity of taking into account the presence of a very large number of ancillary molecules. The situation is rather very similar when one of the phases is solid. Finally, the emergence of reliable theoretical approaches of the innumerable chemical problems encountered in the understanding of living processes is a very promising subject. It generally involves very large molecules such as enzymes or nucleic acids, in which the chemically significant fraction only can be treated at an accurate level and its links with the rest of the macromolecule raise some specific methodological problems.

In this book various aspects of this field in great development are addressed, both from the point of view of the methods and their illustrative applications.

Jean-Louis Rivail
Manuel Ruiz-Lopez
Xavier Assfeld



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Rivail, J.-L.; Ruiz-Lopez, M.; Assfeld, X. (Eds.)

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