

Preface

Quantum chemistry plays a crucial role in many areas of chemistry, physics and biology. There is significant research ongoing in this area of science. International conferences in quantum chemistry are frequently organized in many countries. This book came about as a consequence of the International Symposium “Frontiers of Quantum Chemistry” on November 11, 2015 at Kwansei Gakuin University in Japan.

This book consists of twenty chapters. It presents the frontiers of current research in quantum chemistry in various areas of theory. The chapter topics include: development of correlated single particle theories; density-functional theory; relativistic time-dependent density-functional theory; quantum many-body methods; response theory; SACCI methodology; electron communications theory; vibrational linear and nonlinear optical properties theory; and molecular dynamics. Other chapter topics include: applications in kinetics; description of molecular properties and chemical reactions; nonlinear optical properties in ultraviolet spectroscopy; circular dichroism; nuclear quantum effect and H/D isotope effect in hydrogen-bonded systems; properties of periodic materials subjected to external electric and magnetic fields; photoisomerization reactions; chemical enhancement of surface-enhanced Raman spectroscopy; NIR spectroscopy; and spectroscopy of hydrogen-bonded systems.

The first fourteen chapters, representing the first part of the book, present newly developed methods which might play important roles in future spectroscopic studies. The presented methods elucidate state-of-the-art modern quantum chemistry. It should be pointed out that these chapters revolve around different approaches. Concepts based on the post-Hartree-Fock methods are presented as well as those based on density functional theory. Several chapters are concerned with vibrational linear and nonlinear optical properties which represent modern spectroscopic analysis. Some of the chapters go beyond currently used methods, such as electron communications theory. The second part of the book is devoted to discussions about the applications of current methods. These six chapters cover the most significant and important applications across several fields of science. The application of molecular dynamics simulations for large systems looks very

promising. Determination of isotope effects, as well as reaction mechanism studies, are also essential applications, especially in computational enzymology and biology. These chapters represent a complete source of quantum chemistry knowledge.

We hope readers of this book will learn a great deal about the current state of quantum chemistry and its applications and importance in basic and applied science.

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