Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology

Progress in Theoretical Chemistry and Physics

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Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology

Springer

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PTCP Aim and Scope

Progress in Theoretical Chemistry and Physics

A series reporting advances in theoretical molecular and material sciences, including theoretical, mathematical and computational chemistry, physical chemistry and chemical physics and biophysics.

Aim and Scope

Science progresses by a symbiotic interaction between theory and experiment: theory is used to interpret experimental results and may suggest new experiments; experiment helps to test theoretical predictions and may lead to improved theories. Theoretical Chemistry (including Physical Chemistry and Chemical Physics) provides the conceptual and technical background and apparatus for the rationalisation of phenomena in the chemical sciences. It is, therefore, a wide ranging subject, reflecting the diversity of molecular and related species and processes arising in chemical systems. The book series *Progress in Theoretical Chemistry and Physics* aims to report advances in methods and applications in this extended domain. It will comprise monographs as well as collections of papers on particular themes, which may arise from proceedings of symposia or invited papers on specific topics as well as from initiatives from authors or translations.

The basic theories of physics—classical mechanics and electromagnetism, relativity theory, quantum mechanics, statistical mechanics, quantum electrodynamics—support the theoretical apparatus which is used in molecular sciences. Quantum mechanics plays a particular role in theoretical chemistry, providing the basis for the valence theories, which allow to interpret the structure of molecules, and for the spectroscopic models, employed in the determination of structural information from spectral patterns. Indeed, Quantum Chemistry often appears synonymous with Theoretical Chemistry; it will, therefore, constitute a major part of this book series. However, the scope of the series will also include other areas of theoretical chemistry, such as mathematical chemistry (which involves the use of algebra and topology in the analysis of molecular structures and reactions); molecular mechanics, molecular dynamics and chemical thermodynamics, which play an important

role in rationalizing the geometric and electronic structures of molecular assemblies and polymers, clusters and crystals; surface, interface, solvent and solid state effects; excited-state dynamics, reactive collisions, and chemical reactions.

Recent decades have seen the emergence of a novel approach to scientific research, based on the exploitation of fast electronic digital computers. Computation provides a method of investigation which transcends the traditional division between theory and experiment. Computer-assisted simulation and design may afford a solution to complex problems which would otherwise be intractable to theoretical analysis, and may also provide a viable alternative to difficult or costly laboratory experiments. Though stemming from Theoretical Chemistry, Computational Chemistry is a field of research in its own right, which can help to test theoretical predictions and may also suggest improved theories.

The field of theoretical molecular sciences ranges from fundamental physical questions relevant to the molecular concept, through the statics and dynamics of isolated molecules, aggregates and materials, molecular properties and interactions, to the role of molecules in the biological sciences. Therefore, it involves the physical basis for geometric and electronic structure, states of aggregation, physical and chemical transformations, thermodynamic and kinetic properties, as well as unusual properties such as extreme flexibility or strong relativistic or quantum-field effects, extreme conditions such as intense radiation fields or interaction with the continuum, and the specificity of biochemical reactions.

Theoretical Chemistry has an applied branch (a part of molecular engineering), which involves the investigation of structure-property relationships aiming at the design, synthesis and application of molecules and materials endowed with specific functions, now in demand in such areas as molecular electronics, drug design or genetic engineering. Relevant properties include conductivity (normal, semi- and super-), magnetism (ferro- and ferri-), optoelectronic effects (involving nonlinear response), photochromism and photoreactivity, radiation and thermal resistance, molecular recognition and information processing, biological and pharmaceutical activities, as well as properties favouring self-assembling mechanisms and combination properties needed in multifunctional systems.

Progress in Theoretical Chemistry and Physics is made at different rates in these various research fields. The aim of this book series is to provide timely and in-depth coverage of selected topics and broad-ranging yet detailed analysis of contemporary theories and their applications. The series will be of primary interest to those whose research is directly concerned with the development and application of theoretical approaches in the chemical sciences. It will provide up-to-date reports on theoretical methods for the chemist, thermodynamician or spectroscopist, the atomic, molecular or cluster physicist, and the biochemist or molecular biologist who wish to employ techniques developed in theoretical, mathematical and computational chemistry in their research programs. It is also intended to provide the graduate student with a readily accessible documentation on various branches of theoretical chemistry, physical chemistry and chemical physics.

Preface

This volume collects 20 selected papers from the scientific contributions presented at the Seventeenth International Workshop on Quantum Systems in Chemistry and Physics (and Biology), QSCP-XVII, which was organized by Prof. Matti Hotokka at Åbo Akademi University, Turku, Finland, from August 19 to 25, 2012. Over 120 scientists from 27 countries attended this meeting. Participants of the QSCP-XVII workshop discussed the state of the art, new trends, and future evolution of methods in molecular quantum mechanics, as well as their applications to a wide variety of problems in chemistry, physics, and biology.

The large attendance attained in this conference was particularly gratifying. It is the renowned interdisciplinary character and friendly atmosphere of QSCP meetings that makes them so successful discussion forums.

Turku is located in the southwestern part of Finland. It was the capital city of the country as well as its religious and cultural center throughout the Swedish period. Christina, Queen of Sweden, founded the Åbo Akademi University in Turku in 1630. When Finland became a Grand Duchy under Alexander I, Czar of Russia, in 1809, the former University was transferred to the new capital, Helsinki, and eventually became the University of Helsinki.

The present-day Åbo Akademi University was founded in 1918, shortly after Finland became independent from Russia. Some of the buildings of the old Åbo Akademi University, such as the Ceremonial Hall, are still used by the University. Today, Turku is the seat of the Archbishop of Finland and an active cultural and industrial city endowed with numerous museums, art galleries and historical sites, as well as an important seaport.

Details of the Turku meeting, including the scientific program, can be found on the web site: http://www.qscp17.fi. Altogether, there were 19 morning and afternoon sessions, where 56 plenary talks were given, and one evening poster session, with 21 flash presentations for a total of 55 posters displayed. We are grateful to all participants for making the QSCP-XVII workshop such a stimulating experience and great success.

QSCP-XVII followed the traditions established at previous workshops:
QSCP-I, organized by Roy McWeeny in 1996 at San Miniato (Pisa, Italy);

QSCP-II, by Stephen Wilson in 1997 at Oxford (England);
QSCP-III, by Alfonso Hernandez-Laguna in 1998 at Granada (Spain);
QSCP-IV, by Jean Maruani in 1999 at Marly-le-Roi (Paris, France);
QSCP-V, by Erkki Brändas in 2000 at Uppsala (Sweden);
QSCP-VI, by Alia Tadjer in 2001 at Sofia (Bulgaria);
QSCP-VII, by Ivan Hubac in 2002 near Bratislava (Slovakia);
QSCP-VIII, by Aristides Mavridis in 2003 at Spetses (Athens, Greece);
QSCP-IX, by Jean-Pierre Julien in 2004 at Les Houches (Grenoble, France);
QSCP-X, by Souad Lahmar in 2005 at Carthage (Tunisia);
QSCP-XI, by Oleg Vasyutinskii in 2006 at Pushkin (St Petersburg, Russia);
QSCP-XII, by Stephen Wilson in 2007 near Windsor (London, England);
QSCP-XIII, by Piotr Piecuch in 2008 at East Lansing (Michigan, USA);
QSCP-XIV, by Gerardo Delgado-Barrio in 2009 at El Escorial (Madrid, Spain);
QSCP-XV, by Philip Hoggan in 2010 at Cambridge (England);
QSCP-XVI, by Kiyoshi Nishikawa in 2011 at Kanazawa (Japan).

The lectures presented at QSCP-XVII were grouped into nine areas in the field of *Quantum Systems in Chemistry, Physics, and Biology*, ranging from Concepts and Methods in Quantum Chemistry and Physics through Molecular Structure and Dynamics, Reactive Collisions, and Chemical Reactions, to Computational Chemistry, Physics, and Biology.

The width and depth of the topics discussed at QSCP-XVII are reflected in the contents of this volume of proceedings in the book series *Progress in Theoretical Chemistry and Physics*, which includes four sections:

I. Fundamental Theory (4 papers);
II. Molecular Structure, Properties and Processes (5 papers);
III. Clusters and Condensed Matter (9 papers);
IV. Structure and Processes in Biosystems (2 papers).

In addition to the scientific program, the workshop had its usual share of cultural events. There was an entertaining concert by a tuba orchestra on the premises. The City of Turku hosted a reception on the museum sail ship Suomen Joutsen, and one afternoon was devoted to a visit to the archipelago on board of the old-fashioned steamship Ukkopekka. The award ceremony of the CMOA Prize and Medal took place in the historical Ceremonial Hall of the old Åbo Akademi University.

The CMOA Prize was shared between two selected nominees: Marcus Lundberg (Uppsala, Sweden) and Adam Wasserman (Purdue, USA). The CMOA Medal was awarded to Pr. Martin Quack (ETH, Switzerland). Following an established custom at QSCP meetings, the venue of the next (XVIIIth) workshop was disclosed at the end of the banquet: Paraty (Rio de Janeiro), Brazil, in December 2013.

We are pleased to acknowledge the generous support given to the QSCP-XVII conference by the Federation of Finnish Learned Societies, the Svenska Tekniska Vetenskaps-Akademien i Finland, the City of Turku, the Åbo Akademi University, the Walki company, and Turku Science Park. We are most grateful to the members of the Local Organizing Committee (LOC) for their work and dedication, which made the stay and work of the participants both pleasant and fruitful. Finally, we

would like to thank the members of the International Scientific Committee (ISC) and Honorary Committee (HC) for their invaluable expertise and advice.

We hope the readers will find as much interest in consulting these proceedings as the participants in attending the meeting.

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