

# Topics in the Theory of Chemical and Physical Systems

Proceedings of the 10th European Workshop  
on Quantum Systems in Chemistry and Physics  
held at Carthage, Tunisia, in September 2005

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## **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*

### **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 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, and 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 transformation, 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 supra-), magnetism (ferro- or ferri-), optoelectronic effects (involving nonlinear response), photochromism and photoreactivity, radiation and thermal resistance, molecular recognition and information processing, and 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 fields of research. 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 wishes to employ techniques developed in theoretical, mathematical or computational chemistry in his research programme. 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.

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## PREFACE

This volume contains a representative selection of papers presented at the *Tenth European Workshop on Quantum Systems in Chemistry and Physics* (QSCP-X), held at *Beit al-Hikma*, seat of the *Académie Tunisienne des Sciences, des Arts et des Lettres*, in Carthage, Tunisia, September 1-7, 2005. About 90 scientists from 18 countries, half of them from North Africa, attended the meeting, which focused on the evolution of current issues and problems in methods and applications.

This workshop continued the series that was established by Roy McWeeny near Pisa (Italy), in April 1996, then continued on a yearly basis: Oxford (1997), Granada (1998), Paris (1999), Uppsala (2000), Sofia (2001), Bratislava (2002), Athens (2003), Grenoble (2004) .... The purpose of QSCP workshops is to bring together chemists and physicists with a common field of interest – the quantum mechanical theory of the many-body problem – and foster collaboration at the fundamental level of innovative theory and conceptual development. Quantum mechanics provides a theoretical foundation for our understanding of the structure and properties of atoms, molecules and the solid state in terms of their component particles, electrons and nuclei. The study of ‘Quantum Systems in Chemistry and Physics’ therefore underpins many of the emerging fields in science and technology: nanostructures, smart materials, drug design, and so on.

The tenth workshop was the first in the series held outside Europe. Participants gathered on the coast of North Africa, in one of the most influential cities of the ancient world, Carthage. Founded by Phoenicians from Tyre in the ninth century BC, it challenged the power of Rome. The situation of *Beit al-Hikma* on the Gulf of Tunis provided an excellent venue for scientists from different scientific and cultural backgrounds. They came from Western and Eastern Europe and North and South America as well as from Algeria, Morocco and, of course, Tunisia. Participants from overseas discovered a young and vibrant local scientific community engaged in theoretical molecular physics and chemistry.

The Carthage QSCP workshop was divided into 5 morning and 3 afternoon plenary sessions, during which a total of 36 lectures of about 30 minutes each, including discussion, were delivered by leading experts. There were also 2 evening sessions where 63 posters were presented, each being first described in a 3-minute oral presentation.

The fifteen papers collected in this volume are gathered into three sections, each addressing different aspects of the study of quantum systems in chemistry and physics. They are:

**Part I: Advanced Methodologies**

**Part II: Interactions and Clusters**

**Part III: Excited States and Condensed Matter**

We are pleased to acknowledge the support given to the Carthage workshop by the *University of Tunis*, the *Société Tunisienne d'Optique* and the *Académie Tunisienne des Sciences, des Arts et des Lettres*. The efforts of all members of the Local Organizing Committee were very much appreciated, especially the team of LSAMA (Laboratoire de Spectroscopie Atomique, Moléculaire et Applications), led by Pr Zohra Ben Lakhdar, including Drs Hassen Ghalila, Zoubeida Dhaouadi and Nejmeddine Jaidane. The material and logistic help of the *Tunisian Academy* and of the *Hotel Amilcar* is also gratefully acknowledged.

We are grateful to the participants not only for the high standard of the talks and posters presented at the workshop, which is reflected in this proceedings volume, but also for the friendly and constructive atmosphere throughout the formal and informal sessions. The QSCP workshops continue to provide a unique forum for the presentation and discussion of new ideas and developments.

As usual, since the 2001 workshop in Sofia, an impressive ceremony took place at the banquet dinner, held at the *Hotel Amilcar* in Carthage. The *Promising Scientist Prize* of the *Centre de Mécanique Ondulatoire Appliquée* (PSP of CMOA) was shared between the two selected nominees: Dr Majdi Hochlaf and Dr Richard Taïeb: <http://www.lcpmr.upmc.fr/prize.html>.

We hope that this volume has captured some of the excitement and enthusiasm that participants showed during the QSCP-X workshop, and that it will convey to a wider audience some of the concepts and innovations considered at *Beït al-Hikma*.

**Souad Lahmar**

**Jean Maruani**

**Stephen Wilson**

**Gerardo Delgado-Barrio**



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