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Preface

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## PREFACE

This volume collects 11 selected papers from the scientific contributions presented at the *Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX)*, organized by the team led by Professor Mark Hoffmann at the University of North Dakota, Grand Forks, North Dakota, U.S.A., from July 17 to 22, 2016. The ISTCP-IX Congress in Grand Forks followed the format established at the eight previous meetings:

ISTCP-I:	Professor Ramon Carbo-Dorca, Girona (Spain), June 28 - July 3, 1993
ISTCP-II:	Professor Sean P. McGlynn, New Orleans (LA, USA), April 9 - 13, 1996
ISTCP-III:	Professor Miguel Castro, Mexico City (DF, Mexico), November 8 - 13, 1999
ISTCP-IV:	Professor Jean Maruani, Marly-le-Roi (Paris, France), July 9 - 16, 2002
ISTCP-V:	Professor Peter Politzer, New Orleans (LA, USA), July 20 - 26, 2005
ISTCP-VI:	Professor Yan Alexander Wang, Vancouver (BC, Canada), July 19 - 24, 2008
ISTCP-VII:	Professor Hiromi Nakai, Waseda (Tokyo, Japan), September 2 - 8, 2011
ISTCP-VIII:	Professor Péter Surján, Eötvös (Budapest, Hungary), August 25 - 31, 2013.

The 2016 venue offered the possibility for the approximately 300 participants from 26 countries to join the Congress. Speakers from each of the countries were joined by students from 9 countries. Despite being nearly 2000 km from any sea coast (1200 km, if one counts the Arctic Ocean outlet Hudson Bay), this Congress continued to reflect the strong international characteristics of ISTCP. Countries sending 4 or more delegates include China, Denmark, France, Germany, Hungary, Israel, Japan, Mexico, Netherlands, Norway, Switzerland, and the United Kingdom, besides the U.S.A.

The *International Society for Theoretical Chemical Physics*, ISTCP, was founded in 1990 by Professor János Ladik at the University of Erlangen, Germany. ISTCP has the objectives to promote theoretical developments at the frontier between physics and chemistry. Additionally the goal is to allow younger researchers to interact with leading contributors of the field at regularly organized International Congresses. The Society involves an Honorary Board, a Board of Directors gathering together about 60 scientists (including 5 Nobel Laureates and 2 Wolf Prize laureates) in the fields of Theoretical Chemistry and Physics, and a Board of National Representatives covering about 35 countries/regions. The current President, since July 2000, is Professor Erkki J. Brändas, from Uppsala University, Sweden.

ISTCP Congress Proceedings have been published regularly in the special issues of the *International Journal of Quantum Chemistry (IJQC)* and partly (2002, 2008) co-published in special volumes of *Progress in Theoretical Chemistry and Physics (PTCP)*. Following this tradition, a small and highly targeted set of articles were solicited from researchers in several forefront fields represented at ISTCP IX. These 11 articles are divided into 4 reviews, 3 tutorial reviews, 2 perspectives and 2 papers.

ISTCP-IX was organized into 9 thematic Symposia, plus a special symposium honouring Per-Olov Löwdin. The co-organizers of each of the symposia had significant latitude in inviting leading scientists in their areas, with attention paid to overall geographical, career stage and gender diversity. Moreover, in an effort to stimulate conversation and cross-disciplinary inquiries, each speaker was limited to only 1 talk, and there were never more than 3 parallel sessions. It is the careful thought and hard work of the Symposium Organizers that contributed to the success of the Congress. The Symposia and their Organizers are:

1. Accurate Thermochemistry (Angela Wilson, Branko Ruscic)
2. Chemical Insights (Paul Ayers, Pedro Salvador)

3. Complex Systems (Jiali Gao, Nandini Ananth)
4. Dynamics (George Schatz, Keli Han)
5. Electronic Structure (Piotr Piecuch, Jiri Pittner)
6. Subsystems in Density Functional Theory (Tomasz Wesolowski, Christoph Jacob)
7. Emerging Methods for Quantum N-body Problem (Seiichiro Ten-no, Edward Valeev)
8. Molecular Properties (Trygve Helgaker)
9. Per-Olov Löwdin Symposium (Erkki Brändas)
10. Relativistic Methods (Wenjian Liu, Jochen Autschbach)

In addition to symposia, there were 9 plenary talks for which all participants were gathered. The early and enthusiastic support of the plenary speakers were critical to providing high visibility for the conference, and we are grateful to them.

1. Kim Baldridge, *Structure-Property Relationships of Curved Aromatic Materials from First Principles*
2. Ria Broer, *Theoretical and Computational Studies for the Design of Organic Photovoltaic Materials*
3. Benedetta Mennucci, *Ab Initio Simulation of the Optical Spectroscopy of Multichromophoric Systems*
4. William Miller, *Symmetrical Quasi-Classical Model for Classical Molecular Dynamics Simulations of Electronically Non-adiabatic Processes*
5. Debashis Mukherjee, *A Survey of the Unitary Group Adapted MRCC and MRPT Theories: SU vs SS Approaches*
6. Martin Quack, *The Quantum Dynamics of Chiral and Achiral Molecules including Electroweak Parity Violation: Theory and Experiment*
7. Andreas Savin, *Multireference Density Functional Theory*
8. Henry F. Schaefer III
9. Tamar Seideman, *Coherent Alignment in Complex Systems*

This Preface does not allow a comprehensive account of all the excellent contributions to the conference or to the articles submitted to these proceedings. The 4 Reviews consider relativistic treatment of molecular properties, charge transfer in molecular crystals and in organic polymeric materials, and advances in subsystem embedding. These are complemented by Tutorial Reviews on molecular motors, the inverse approach to exchange-correlation potentials, and the random phase approach in the context of reduced density matrices. One full paper considers the chemistry of new super heavy elements and the other on data considerations in petascale computations of chemical and biological systems. There are Perspectives on non-collinear electronic structure calculations and calculations of atoms and molecules in strong magnetic fields. The articles in the proceedings can be grouped roughly into extension of theory and calculations into much larger systems than could be considered just a few years ago and extension of precision in theory and calculations.

We are grateful to all organizers for their exceptional work. In particular we want to thank Professor Janos Ladik, Founder of the Society and Honorary Chair. We were sorry to learn that he could not participate in person but his kind interest and strong support in the various matters of the venue were indeed a positive factor. We are indebted to our excellent organizing committee that guided us in producing a well-balanced, global perspective on cutting-edge chemical physics: Gustavo Aucar, T. Daniel Crawford, Peter Gill, Anna Krylov, Hiromi Nakai, Katarzyna Pernal, Péter Surján and Ágnes Szabados. We are also grateful to all session chairs, speakers, poster presenters, as well as all student volunteers, contributing significantly to the great success of the meeting. For more details regarding the Congress we refer to our web site <http://istcp-2016.org/>.

The ISTCP-IX Congress took place at the Alerus Center, near the University of North Dakota campus. The assistance of the staff at the Alerus Center and at the Greater Grand Forks Convention

and Visitors Bureau were critical in facilitating an event of this complexity in this city of only 60,000 people. But, most of all, it was the unwavering support of former UND President Robert Kelley, Vice President of Academic Affairs and Provost Tom DiLorenzo, Vice President for Research and Economic Development Grant McGimpsey, and Division of Research Staff Cathy Lerud and Carla Kellner that made this happen.

We are pleased to express our sincere thanks to our sponsors. In addition to generous support from the University of North Dakota and the Greater Grand Forks Convention and Visitors Bureau, which allowed low-cost registration and accommodations for students, we are pleased to be able to acknowledge additional support from Physical Chemistry Chemical Physics and Department of Energy. These contributions from our sponsors have enabled us to maintain the high-quality standard of the Congress.

The guest editors of this Special Issue, finally, want to thank the authors, who accepted our invitation to contribute to these proceedings, and in so doing provide a perspective of some cutting edge areas of inquiry in chemical physics. The IXth Congress of ISTCP included both these areas and many more. We hope that all researchers with a great interest in theory and methods related to fundamental scientific problems and future progress of our field will appreciate this volume.

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