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## PREFACE

This volume collects 32 selected papers from the scientific contributions presented at the *Eighth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VIII)*, organized by the team led by Professor Péter Surján at Eötvös University, Budapest, Hungary, from August 25 to 31, 2013. The ISTCP-VIII Congress in Budapest followed the format established at the seven 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.

The 2013 venue offered the possibility for the 358 registered participants from 41 countries to join the Congress. The participation statistics, shown below, clearly reflects the strong international characteristics of ISTCP. Countries sending 7 or more delegates are named explicitly.

Hungary 47	Japan 39	USA 38	Germany 37	Poland 21	Czech Republic 14
France 13	Sweden 11	Russia 10	Canada 9	China 9	India 9
UK 9	Denmark 8	Spain 8	Belgium 7	Israel 7	Other countries 62

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, the present issue collects selected Perspectives (12), Full Papers (15), Review Articles, including Tutorial Reviews (5) from invited oral speakers at the Congress, thereby reflecting the various fields covered by ISTCP VIII.

At ISTCP-VIII, three Congress Lectures were organized:

Peter Pulay:	<i>Ultrafast Quantum/Molecular Mechanics Monte Carlo Simulations</i>
Gustavo Scuseria:	<i>Symmetry Breaking and Restoration</i>
Ingvar Lindgren:	<i>Development of Many-Body Perturbation Theory: How to combine with Quantum ElectroDynamics</i>

The Congress also included 190 Lectures, and 154 Poster Presentations.

The following oral sessions were thematized under the headings:

1. Biological Applications
2. Can we See the Forest for the Trees? - Interpretation Models in Quantum Chemistry
3. Electron Correlation - In Memoriam Isaiah Shavitt
4. London Dispersion Forces in Electronic Structure Theory
5. Fragment Approach and Electron Localization in Quantum Chemistry
6. Fundamental Problems in Quantum Chemistry
7. Molecular Dynamics - from quantum dynamics to mesoscale dynamics
8. Relativistic Effects in Molecules
9. Solid State Chemistry
10. Uncertainty Quantification in Chemical Kinetics and Thermodynamics

In addition, several non-thematical sessions were organized with leading scientists as invited speakers.

The ISTCP-VIII Congress took place at the Budapest Congress Center, on the Buda side of Budapest. Accompanying persons attended specially organized social events such as a Dinner Cruise on the river Danube, an excursion to the Northwestern region of Hungary, visiting Pannonhalma, Sopron, Fertőd and enjoying Hungarian culture at its best.

This Preface does not allow a comprehensive account of all the excellent contributions submitted to these proceedings. Nevertheless the field of Chemical Physics is here covered by 12 Perspectives, starting with quantum chemistry and its ages, recounting fundamental problems via chemical reaction dynamics, multi-reference perturbation theories, nano-particle reactivity, various materials design to the present standing of relativistic Hamiltonian formulations. The full papers treated novel method developments like recent time- and time-independent Density Functional Theory, Double hybrid DFT, Coulomb bipolar expansions, Quantum Monte Carlo applications, and hot topics like the physical and chemical nature of graphene, and the biological onset of cancer. A number of extraordinary Reviews reconsider the chemical physics of unconventional superconductivity, analytic energy derivatives in relativistic quantum chemistry and the development of many-body theory in combination with quantum electro dynamics.

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. Most of all we are indebted to our excellent leaders of the Thematic Sessions: Lyudmila Slipchenko, Peter Gill, Mihály Kállay, János Ángyán, Shuhua Li, Cleanthes A. Nicolaidis, Kersti Hermansson, Jürgen Gauss, Miklós Kertesz, and Tamás Turányi. We are also grateful to all session chairs, speakers, poster presenters, as well as all participants of the congress, contributing significantly to the great success of the meeting. For more details regarding the Congress we refer to our web site <http://coulson.chem.elte.hu/istcp8/>

We are pleased to express our sincere thanks to our sponsors: the Gedeon Richter and the EGIS Pharmaceuticals companies, who supported participant costs for young researchers and students, and the Foundation for Chemistry Education at Eötvös University, Budapest, who provided parts of the accommodation and registration fees for students. The Springer Company offered two poster prizes targeting also young participants. 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 displayed an appropriate cross-section of the VIIIth Congress of ISTCP. 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.

Erkki Brändas  
Ágnes Szabados  
Péter Surján