THE VIIITH CONGRESS OF THE

INTERNATIONAL SOCIETY FOR

THEORETICAL CHEMICAL PHYSICS

PROGRAM

25-31 AUGUST 2013, BUDAPEST

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Program

25/08 Sunday

Hall Pátria **Opening**

17:00 – 17:30 **Péter Surján, Erkki Brändas**

Congress Service Area **Welcome Reception**

19:00 –

26/08 Monday Morning I

Hall Pátria Chair: **Ingvar Lindgren** **Congress Talk**

8:30 – 9:20 Gustavo Scuseria
Symmetry Breaking and Restoration

Hall Pátria Chair: **Jürgen Gauss** **Relativistic Effects in Molecules**

9:30 – 10:00 Stella Stopkowicz
Does Direct Perturbation Theory converge?

10:00 – 10:30 Werner Kutzelnigg
The no-photon approximation in relativistic quantum chemistry

Room Bartók Chair: **Lyudmila Slipchenko** **Biological Applications**

9:30 – 10:00 Lyudmila Slipchenko
Hybrid quantum/classical and fragmentation techniques for radicals and electronic excited states

10:00 – 10:30 Jan Halborg Jensen
Quantum Biochemistry

26/08 Monday Morning I cont'd

Room Lehár Chair: **Kresimir Rupnik** **Versatile Topics**

9:30 – 9:50 Dominika Zgid
How to make Dynamical Mean Field Theory quantitative?

9:50 – 10:10

10:10 – 10:30 Monika Musial
Multireference Fock space coupled cluster method based on the RHF reference for the description of the potential energy curves

coffee break

26/08 Monday Morning II

Hall Pátria Chair: **Jürgen Gauss** **Relativistic Effects in Molecules**

11:00 – 11:30 Wenjian Liu
Fundamentals of Relativistic Molecular Quantum Mechanics

11:30 – 12:00 Dieter Cremer
Calculation of response properties with the normalized elimination of the small component (NESC) method

12:00 – 12:30 Lan Cheng
Cost-effective approaches for relativistic electron-correlated calculations

Room Bartók Chair: **Lyudmila Slipchenko** **Biological Applications**

11:00 – 11:30 Qiang Cui
QM/MM analysis of catalytic promiscuity and proton pumping in enzymes

11:30 – 11:50 Magdalena Pecul
Calculations of circular dichroism and circularly polarized luminescence spectra of biologically relevant chromophors.

11:50 – 12:10 Erik Donovan Hedegård
Polarizable Embedding: Multireference embedding methods and large scale applications to optical properties in proteins

12:10 – 12:30 Edina Rosta
Two-Metal Ion Catalysis by Ribonuclease H

26/08 Monday Morning II cont'd

Room Lehár Chair: **Katarzyna Pernal** **Versatile Topics**

11:00 – 11:30 Petr Carsky
Evaluation of exchange integrals by Fourier transform of the $1/r$ operator and its numerical quadrature

11:30 – 11:50 Ors Legeza
Generalized tensor methods and entanglement measurements for electronic structure calculations

11:50 – 12:10 Feiwu Chen
A new size extensive multireference perturbation theory

12:10 – 12:30 Elvira Romera
Phase-space visualization of quantum phase transitions in the molecular vibron model

lunch break

26/08 Monday Afternoon I

Hall Pátria Chair: **Wenjian Liu** **Relativistic Effects in Molecules**

14:30 – 15:00 Pekka Pyykkö
Aspects of accurate, relativistic quantum chemical calculations

15:00 – 15:30 Trond Saue
The relativistic correlation problem

15:30 – 16:00 Ria Broer
The Combined Effects of Electron Correlation and Relativity on Core Excitation Spectra

16:00 – 16:20 Artur Wodyński
The influence of a presence of a heavy atom on spin-spin coupling constants between two light atoms in organometallic compounds and halogen derivatives

Room Bartók Chair: **Lyudmila Slipchenko** **Biological Applications**

14:30 – 15:00 Dennis Salahub
Towards the multiscale modeling of catalysis

15:00 – 15:20 Gábor Náray-Szabó
Mechanism of enzymatic phosphate ester hydrolysis: interplay of theory and experiment

15:20 – 15:40 Marc de Wergifosse
Theoretical investigation of the second-order nonlinear optical response of collagen – signatures of the triple helix structure

15:40 – 16:00 Andrzej Sokalski
Modeling of enzymatic organophosphate hydrolysis: towards design of new biocatalysts

16:00 – 16:20 Kresimir Rupnik
Adaptive UF PPS Model Study of Structures and Reactions in Biomolecules: New Selective Bio-Molecular Probes through High Magnetic Fields

26/08 Monday Afternoon I cont'd

Room Lehár Chair: **Miroslav Urban** **Versatile Topics**

14:30 – 15:00 György Lendvay
Barrier evasion and roaming in the dynamics of elementary chemical reactions

15:00 – 15:20 Kirill Gokhberg
Decay processes mediated by long-range electron correlation

15:20 – 15:40 Jing Ma
Reactive molecular dynamics simulations of switching processes of azobenzene-based monolayer on surface

15:40 – 16:00 Kenneth Ruud
Analytic DFT calculations of anharmonic force constants

16:00 – 16:20 Roberto Cammi
Harmonic vibrational frequencies in molecules at extreme high pressure: a novel QM method

coffee break

Hall Pátria Chair: **Gustavo Scuseria** **Congress Talk**

16:50 – 17:40 Peter Pulay
Ultrafast Quantum/Molecular Mechanics Monte Carlo Simulations

26/08 Monday Evening

Aula **Poster Session I**

18:00 – 20:00

27/08 Tuesday Morning I

Room Bartók Chair: **Peter Gill** **Interpretation Models in Quantum Chemistry**

8:30 – 9:00 Peter Gill
An interpretive dance in three movements

9:00 – 9:30 Axel Becke
Two-Determinant Mixing with a Strong-Correlation Density Functional

9:30 – 9:50 Kristine Pierloot
Electronic structure of manganese(II) nitrosyl compounds: a bifocal view

9:50 – 10:10 Shmuel Zilberg
Chemical Reactions with two different elementary Transition States – Crypto Three-State System. Photo-/ Thermo-chemical aspects and VB rationalization.

10:10 – 10:30 Takao Tsuneda
A reactivity index based on orbital energies

Room Lehár Chair: **Miklos Kertesz** **Solid State Chemistry**

8:30 – 9:00 Sumit Mazumdar
Superconductivity as a problem in chemical physics

9:00 – 9:30 Claudia Draxl
From structure to opto-electronic excitations of organic-inorganic hybrid materials: State of the art and challenges

9:30 – 9:50 An Ghysels
Thermodynamics of framework breathing: free energy model for flexible porous crystals

9:50 – 10:10 Miroslav Urban
CCSD(T) calculations of confined systems: In crystal polarizabilities of anions

10:10 – 10:30 Benoît Champagne
Towards calculating and interpreting the linear and second-order non-linear optical properties of molecular crystals

Room Brahms Chair: **Tamás Turányi** **Uncertainty Quantification**

8:30 – 9:00 Tamás Turányi
Quantification of the Uncertainty of Parameters in Chemical Kinetics

9:00 – 9:30 Michael Frenklach
UQ-Predictive Modeling of Chemical Reaction Systems

9:30 – 10:00 Judit Zádor
Uncertainties in ab initio rate coefficient calculations

10:00 – 10:30 Hai Wang
Multiscale Kinetic Knowledge Propagation – Combustion Chemistry of Small Hydrocarbons

coffee break

27/08 Tuesday Morning II

Room Bartók Chair: **Peter Gill** **Interpretation Models in Quantum Chemistry**

11:00 – 11:30 Weitao Yang
Exchange-Correlation Energies from Paring Matrix Fluctuation and Particle-Particle-Random Phase Approximation

11:30 – 11:50 Elfi Kraka
The decisive role of hydrogen-bonds in chiral discrimination - unraveled by quantum chemical means

11:50 – 12:10 Avital Shurki
Insights on Enzyme Catalysis

12:10 – 12:30 Jeng-Da Chai
Restoration of the Derivative Discontinuity in Kohn-Sham Density Functional Theory: An Efficient Scheme for Energy Gap Correction

Room Lehár Chair: **Miklos Kertesz** **Solid State Chemistry**

11:00 – 11:30 Nicola Marzari
The density is not enough

11:30 – 11:50 Kersti Hermansson
Ceria chemistry at the nano-scale

11:50 – 12:10 Karoly Nemeth
Quantum-chemical Design of Improved Photoemissive Materials

12:10 – 12:30 Mazharul M. Islam
Theoretical study for lithium diffusion in $Li_2Ti_xO_y$ compounds

Room Brahms Chair: **Tamás Turányi** **Uncertainty Quantification**

11:00 – 11:30 David Sheen
Uncertainty Quantification and Data Discrimination in Combustion Kinetic Modeling

11:30 – 11:50 Carsten Olm
Uncertainty of the rate parameters in the wet CO combustion system

11:50 – 12:10 Elke Goos
Evaluation of the influence of thermodynamic data on the Prediction of propane and propene ignition delay times

12:10 – 12:30 Tibor Furtenbacher
Graph theory in spectroscopy and thermochemistry

lunch break

27/08 Tuesday Afternoon I

Room Bartók Chair: **Peter Gill** **Interpretation Models in Quantum Chemistry**

14:30 – 15:00 Gernot Frenking
Main Group Complexes with Unusual Donor-Acceptor Bonds

15:00 – 15:30 Andreas Savin
Getting to Lewis electron pairs from quantum mechanical calculations: Maximum Probability Domains

15:30 – 15:50 Marco Nascimento
Quantum Interference Provides a Unified Description of Chemical Bonding

15:50 – 16:10 Peter Karadakov
Magnetic Shielding as a Source of Information about Aromaticity, Antiaromaticity and Chemical Bonding

16:10 – 16:30 Tom Ziegler
Analyzing Complex Electronic Structure Calculations on Large Molecules in Simple Chemical Terms

Room Lehár Chair: **Benoît Champagne** **Solid State Chemistry**

14:30 – 15:00 Jean-Francois Halet
Rings and Chains in Solid-State Chemistry. The Electron Count Matters

15:00 – 15:30 Miklos Kertesz
$\pi - \pi$ stacking is different from pancake bonding: interpretations with molecular and solid state examples

15:30 – 15:50 Reinhard Maurer
Towards a mechanistic understanding of photoinduced (non-)switching of metal surface adsorbed Azobenzenes.

15:50 – 16:10 Frantisek Karlicky
The Reaction of Water with Iron: Surface Science by Random Phase Approximation

16:10 – 16:30 Javier Fdez. Sanz
Mechanism of the Water-Gas Shift Reaction at the Metal-Oxide Interface: Insights from First Principles Calculations

27/08 Tuesday Afternoon I cont'd

Room Brahms Chair: **Judit Zádor** **Uncertainty Quantification**

14:30 – 15:00 Branko Ruscic
Active Thermochemical Tables: Uncertainty Quantification in Thermochemistry

15:00 – 15:30 Markus Kraft
Optimisation and Bayesian Parameter Estimation of a Kinetic Model of n-Propylbenzene Oxidation in a Shock Tube

15:30 – 15:50 Fabien Cailliez
Statistical approaches to forcefield calibration and prediction uncertainty in molecular simulation

15:50 – 16:10 Tamas Varga
Uncertainty quantification of the rate parameters of an ethyl iodide pyrolysis mechanism

16:10 – 16:30 Péter Jeszenszki
Sensitivity analysis of state-specific multireference perturbation theory

coffee break

27/08 Tuesday Afternoon II

Room Bartók Chair: **Peter Gill** **Interpretation Models in Quantum Chemistry**

17:00 – 17:30 Jesus Ugalde
Natural Orbital Functional Theory of the Molecular Electronic Structure

17:30 – 18:00 Laszlo v. Szentpaly
Saving Sanderson's Principle? Order of Magnitude Improvements by Equalizing Mulliken Valence-State Electronegativities χ_{VS} Instead of DFT-Based Chemical Potentials μ

18:00 – 18:30 Istvan Mayer
Extracting chemical information from molecular wave functions – some recent results

18:30 – 19:00 Paul Geerlings
The linear response function as an interpretational tool: retrieving atomic shell structure, inductive and mesomeric effects, aromaticity and anti-aromaticity

Room Lehár Chair: **Benoît Champagne** **Solid State Chemistry**

17:00 – 17:30 Kazunari Yoshizawa
Orbital views of molecular conductance and spintronics

17:30 – 18:00 Philip Hoggan
Quantum Monte Carlo making progress with metal surfaces: CO adsorbed on Cu(100) and Pt(100)

18:00 – 18:30 Jenő Kürti
Raman bands in small diameter carbon nanotubes

28/08 Wednesday Morning I

Hall Pátria Chair: **Mihály Kállay** **Electron Correlation – In Memoriam Isaiah Shavitt**

8:30 – 8:40 Mihály Kállay
Introduction

8:40 – 9:10 Poul Joergensen
The divide-expand-consolidat (DEC) coupled cluster method goes massively parallel.

9:10 – 9:40 Hans-Joachim Werner
Explicitly Correlated Multireference Electronic Structure Methods

9:40 – 10:10 Debashis Mukherjee
Unitary Group Adapted Approach to Spin-free Multi-Reference Coupled Cluster Theories: Formalisms and Applications

10:10 – 10:30 Anna Krylov
Resolution-of-Identity and Cholesky Representations of Electron-Repulsion Integrals within Coupled-Cluster and Equation-of-Motion Methods: Go One More Mile

Room Bartók Chair: **Erkki Brändas** **Fundamental Problems in Quantum Chemistry**

8:30 – 9:00 Cleanthes Nicolaides
The Fifth Age of Quantum Chemistry?

9:00 – 9:30 Moshe Shapiro
The quantum dynamics experienced by a single molecular eigenstate excited by incoherent light

9:30 – 10:00 Armin Scrinzi
Formation of doubly excited states by XUV excitation and Auger spectra in presence of strong IR fields

10:00 – 10:30 Ivana Paidarova
Extracting complex resonance energies from real calculations

Room Lehár Chair: **Miguel Castro** **Versatile Topics**

8:30 – 8:50 Elena Sheka
Graphene, Silicene and Forgotten Lessons of Surface Science

8:50 – 9:10 Evgeniy Gromov
Correlation-bound states of C_{60}^- anion

9:10 – 9:30 Joanna Kauczor
Complex polarization propagator: a theoretical study of molecular properties and spectra

9:30 – 9:50 Selma Engin
Probing IR-Raman rovibrationally excited HCl molecule with X-ray spectroscopies : a theoretical approach

9:50 – 10:10 Robert Góra
The Origins of Large Interaction-Induced First Hyperpolarizabilities in Hydrogen-Bonded π-Electronic Complexes

10:10 – 10:30 Irena Efremenko
Ligand effect on the electronic structure and reactivity of rhodium pincer complexes

coffee break

28/08 Wednesday Morning II

Hall Pátria Chair: **Dennis Salahub** **Electron Correlation**

11:00 – 11:30 Péter Szalay
In memoriam Shi Shavitt: Application of MR-CI methods to describe the potential energy surfaces of O_3 and the dimer of O_2

11:30 – 12:00 Paul Ayers
A New Mean-Field Method for Strong Correlation Using Antisymmetric Products of Nonorthogonal Geminals

12:00 – 12:30 Trygve Helgaker
Molecular magnetism and density-functional theory in magnetic fields

Room Bartók Chair: **Cleanthes Nicolaides** **Fundamental Problems in Quantum Chemistry**

11:00 – 11:30 Erkki Brändas
Time's Arrow Revisited

11:30 – 11:50 Peter Saalfrank
Electrons in motion, or: Can we nake a Hartree-Fock state?

11:50 – 12:10 Michael Filatov
Theoretical design of conical intersections in molecular motors and switches: A Density Functional Theory perspective

12:10 – 12:30 Paul Mezey
Macromolecular Conformation Analysis by the LIL-ADMA Method: How to Deal With Many Atoms Moving in All Directions?

Room Lehár Chair: **W. Andrzej Sokalski** **Biological Applications**

11:00 – 11:30 Per Siegbahn
Water oxidation mechanism in photosystem II

11:30 – 12:00 Alexander Nemukhin
Modeling structure and spectra of fluorescent proteins

12:00 – 12:30 Oleg Prezhdo
Nanoscale Carbon for DNA Sequencing and Drug Delivery

lunch break

28/08 Wednesday Afternoon

Hall Pátria Chair: **Jeppe Olsen** **Electron Correlation**

14:30 – 15:00 John Stanton
How much do, and can, we "understand" about the ground state of NO_3

15:00 – 15:30 Frank Neese
Recent development in pair natural orbital based local coupled cluster methods

15:30 – 16:00 Hiromi Nakai
Linear-Scaling Electron-Correlation Theory for Two-Component Relativistic Hamiltonian

Room Bartók Chair: **Jiri Horacek** **Fundamental Problems in Quantum Chemistry**

14:30 – 15:00 Nimrod Moiseyev
Chemistry and Physics in high-frequency strong laser fields

15:00 – 15:20 Hazel Cox
The stability of Coulomb three-body systems

15:20 – 15:40 Harris Silverstone
Convergence of the bipolar expansion for the Coulomb potential

15:40 – 16:00 Henryk Witek
Analytical wave function of helium atom

Room Lehár Chair: **Reinhold Fink** **Versatile Topics**

14:30 – 15:00 Pedro Salvador
Oxidation states from wavefunction analysis

15:00 – 15:20 Masanori Tachikawa
Multi-component molecular methods for hydrogen bonded systems and positronic compounds

15:20 – 15:40 Fedor Naumkin
Molecular vs atomic encapsulation of hydrogen in metal cluster-cage assemblies

15:40 – 16:00 Petra Ruth Kapralova
Gaussian basis sets for complex scaling calculations

Cruising Boat "Európa" **Banquet**

19:00 –

29/08 Thursday Morning I

Room Bartók Chair: **Hans-Joachim Werner** **Electron Correlation**

8:30 – 9:00 Rodney Bartlett
Some Considerations of Electron Correlation Introduced as a Correlation Potential

9:00 – 9:30 Christian Ochsenfeld
Linear- and sublinear-scaling Moeller-Plesset (MP2) and symmetry-adapted perturbation theory (SAPT)

9:30 – 9:50 Karol Jankowski
Unexpected features of correlation effects involving 3d-electrons

9:50 – 10:10 Reinhold Fink
Assessing ab initio methods by analyzing their wave functions

Room Lehár Chair: **Kersti Hermansson** **Molecular Dynamics**

8:30 – 8:40 Kersti Hermansson
Introduction

8:40 – 9:10 Marco Masia
Force Field Parameterization from a Force Matching–like Approach: Merits, Shortcomings and Future Perspectives.

9:10 – 9:40 Bernd Ensing
Ab initio molecular dynamic simulation of photoactive proteins in action

9:40 – 10:10 Gunnar Nyman
Dynamics of chemical reactions in the gas phase

10:10 – 10:30 Andrzej Bil
Modifying the Fullerene Surface Using Endohedral light guests. From Ab Initio Molecular Dynamics and Metadynamics to Quantum Chemical Topology.

29/08 Thursday Morning I cont'd

Room Brahms Chair: **Matthias Ernzerhof** **Versatile Topics**

8:30 – 8:50 Toomas Tamm
Conformations of Small Molecules

8:50 – 9:10 Adel El-Azhary
Conformatonal and Vibrational Analysis of 12-thiacrown-4 and 18-thiacrown-6

9:10 – 9:30 Imre Pápai
Hydrogen activation by frustrated Lewis pairs: Comparison of reactivity models

9:30 – 9:50 Vitaly Kiselev
A Novel Mechanism of Thermal Decomposition of 1,2-Diamino-1,2-Dinitroethylene (FOX-7): New Insights from High-level Quantum Chemical Calculations

9:50 – 10:10 Jan Mitschker
Interaction of water with rutile (110) – Ground and excited states

10:10 – 10:30 Alia Tadjer
Molecular Dynamics Assessment of Concentration- and Head-Size-Dependent Effects on $C_{12}E_x$ Aggregation

coffee break

29/08 Thursday Morning II

Room Bartók Chair: **Debashis Mukherjee** **Electron Correlation**

11:00 – 11:30 Mark Hoffmann
GVVPT2 Descriptions of Electronic Structures of Metalloid Oxides

11:30 – 11:50 Katarzyna Pernal
Electron excitation energies from reduced density matrices: extended random phase approximation and linear response theory approaches

11:50 – 12:10 Jiri Pittner
Recent Progress in Multireference Hilbert-Space Coupled Cluster Methods: Explicit Correlation, Massively Parallel Implementation, and USS Corrections

12:10 – 12:30 Mario Piris
MCPT-PNOF5: A useful method for dealing with strongly correlated systems

29/08 Thursday Morning II cont'd

Room Lehár Chair: **Kersti Hermansson** **Molecular Dynamics**

11:00 – 11:30 Kai Nordlund
Understanding the interaction of energetic particles with fusion reactor first walls: from binary collision physics to bond conjugation chemistry

11:30 – 11:50 Przemyslaw Dopieralski
Mechanochemistry: The curious case of cyclopropane.

11:50 – 12:10 Paweł Artur Siuda
Nucleation and growth of methane clathrate hydrate crystal - molecular dynamics study

12:10 – 12:30 Maxim Tafipolski
Intermolecular Force Field Parameterization from First Principles

Room Brahms Chair: **Petr Carsky** **Versatile Topics**

11:00 – 11:30 Ágnes Vibók
Quantum control by laser-induced conical intersections

11:30 – 11:50 Yasuteru Shigeta
Free energy analyses on cluster deformations by cumulant mechanics

11:50 – 12:10 Masayoshi Nakano
Nonlinear optical properties of asymmetric diradical molecules

12:10 – 12:30 Gábor Magyarfalvi
An intrinsic measure for the reliability of calculated VCD band signatures

lunch break

29/08 Thursday Afternoon I

Room Bartók Chair: **Bogumil Jeziorski** **Electron Correlation**

14:30 – 15:00 Jeppe Olsen
Correlation Methods Using Non-Orthogonal Orbitals

15:00 – 15:30 Vitaly Rassolov
Multireference DFT based on Strongly Orthogonal Geminals

15:30 – 16:00 Piotr Piecuch
Recent progress in the active-space electron-attached and ionized equation-of-motion coupled-cluster methodologies

29/08 Thursday Afternoon I cont'd

Room Lehár Chair: **Kersti Hermansson** **Molecular Dynamics**

14:30 – 15:00 Eckhard Spohr
Molecular dynamics and reactive trajectory approaches to modeling of electrochemical reactions near the liquid/solid interface

15:00 – 15:20 Jayesh Bhatt
Molecular simulations of hydrated inorganic nanopores

15:20 – 15:40 Ben Nebgen
Theoretical investigation of the excited state proton transfer in 3-cyano-6-hydroxycoumarin

15:40 – 16:00 Kaoru Yamazaki
Selective Vibrational Mode Excitation in Nanocarbons by Tailored Intense Near-Infrared Pulses and Subsequent Intramolecular Vibrational Energy Redistributions

Room Brahms Chair: **Mark Hoffmann** **Versatile Topics**

14:30 – 15:00 Attila Bende
Quantum Theoretical Investigation to Explain the Onset of Cancer

15:00 – 15:30 Wesley Allen
Intramolecular Dispersion

15:30 – 16:00 Mikhail Basilevsky
The microscopic model for electron transfer in disordered solid matrices

coffee break

29/08 Thursday Afternoon II

Room Bartók Chair: **Péter Szalay** **Electron Correlation**

16:30 – 17:00 Jozef Noga
Expectation value coupled cluster approach using the ansatz with generalized double-substitutions cluster operator.

17:00 – 17:20 Masato Kobayashi
Geminal-based wavefunction theory and its perturbative improvement

17:20 – 17:40 Roberto Olivares-Amaya
Useful Parameters of DMRG for Everyday Quantum Chemistry Applications

17:40 – 18:00 Koji Ando
Electron Wave Packet Modeling of Chemical Bonding

29/08 Thursday Afternoon II cont'd

Room Lehár Chair: **Kersti Hermansson** **Molecular Dynamics**

16:30 – 17:00 Nikos Doltsinis
Connecting quantum events to macroscopic phenomena: Multiscale simulation of photoresponsive materials

17:00 – 17:20 Maciej Smiechowski
Spatial decomposition and assignment of vibrational spectra: Dipolar coupling and correlated particle motion in aqueous Li^+

17:20 – 17:40 Janos Daru
Rate constants from equilibrium simulations: a new method

17:40 – 18:00 Haibo Ma
Solvent Effects on Electronic Absorption, Fluorescence and Phosphorescence of Acetone and Benzene in Water: A QM/MM Study

29/08 Thursday Evening

Aula **Poster Session II**

18:00 – 20:00

30/08 Friday Morning I

Hall Pátria Chair: **Shuhua Li** **Fragment Approach and Electron Localization**

8:30 – 8:50 Shuhua Li
Cluster-in-molecule local correlation approach

8:50 – 9:20 So Hirata
First-principles prediction of the structures, spectra, and phase diagrams of molecular crystals

9:20 – 9:50 Martin Schuetz
Local correlation methods for molecules and solids

9:50 – 10:10 Ida-Marie Høyvik
Challenges in orbital localization for orthonormal molecular orbitals

10:10 – 10:30 Joachim Friedrich
The incremental scheme for CCSD(T) and CCSD(T)(F12)

29/08 Friday Morning I cont'd

Room Bartók Chair: **Janos Angyan** **London Dispersion Forces**

8:30 – 9:00 Janos Angyan
State-of-the-art and perspectives in modeling of London dispersion forces

9:00 – 9:30 Georg Jansen
Dispersion interactions from intermolecular perturbation theory and random phase approximations

9:30 – 9:50 Emmanuel Fromager
Rigorous formulation of double hybrid density-functionals along the adiabatic connection

9:50 – 10:10 Rafal Podeszwa
Efficient calculations of accurate interaction energies for nano-scale systems

10:10 – 10:30 Glenn Martyna
Towards an accurate treatment of many-body dispersion and polarization for chemical accuracy via a coarse grained Gaussian Electronic Structure

coffee break

30/08 Friday Morning II

Hall Pátria Chair: **So Hirata** **Fragment Approach and Electron Localization**

11:00 – 11:30 Hermann Stoll
Local correlation-energy increments for solids – ground and excited states

11:30 – 12:00 Shridhar Gadre
Molecular Tailoring Approach : An Art of the Possible for ab initio

Room Bartók Chair: **Ágnes Nagy** **London Dispersion Forces**

11:00 – 11:30 Bogumil Jeziorski
Long-range retardation of relativistic interatomic potentials

11:30 – 12:00 John Dobson
Understanding effects beyond pairwise additivity in dispersion interactions

12:00 – 12:30 Alexandre Tkatchenko
(Un)Chemical Bonding: Surprises in Non-Covalent Interactions in Molecular Systems

lunch break

30/08 Friday Afternoon I

Hall Pátria Chair: **Jozef Noga** **Versatile Topics**

14:30 – 15:00 Samantha Jenkins
Concepts of Quantum Geometry from the Topological Origins of QTAIM

15:00 – 15:30 Michael Hanrath
Extending the Domain of Connectivity for MRexpT: Analysis and Results

15:30 – 16:00 Daniel Crawford
Solvation, Coupled Cluster Response Theory, and the Optical Properties of Chiral Molecules

Room Bartók Chair: **Dominika Zgid** **Versatile Topics**

14:30 – 15:00 Ágnes Nagy
Orbital-free density functional theory: functional derivative of the kinetic energy for spherically symmetric systems

15:00 – 15:30 Matthias Ernzerhof
New functionals through factorization of the exchange and exchange-correlation hole

15:30 – 15:50 Miguel Castro
Theoretical Study of Fe-$(H_2O)_m$, $m < 4$ and Fe_n-$(C_6H_6)_m$, n <7 , m <4.

coffee break

30/08 Friday Afternoon II

Hall Pátria Chair: **Karol Jankowski** **Versatile Topics**

16:30 – 17:00 Josef Michl
Accommodation of Electronic Excitation in sigma-Bond Systems: Peralkylated Oligosilanes

17:00 – 17:30 Pavel Hobza
How accurate are „gold standard“ CCSD(T)/CBS interaction energies?

Hall Pátria Chair: **Peter Pulay** **Congress Talk**

17:40 – 18:30 Ingvar Lindgren
Development of Many-Body Perturbation Theory: How to combine with Quantum ElectroDynamics

Hall Pátria **Closing**

18:30 – 19:00

Papers in Poster Session I

No.	Name	Title
1	Matthew Addicoat	Stochastic Structure Determination for Conformationally Flexible Clusters: CrazyLego
2	Christoph Allolio	An Ab Initio Microscope: Molecular Contributions to the Femtosecond Time-Dependent Fluorescence Shift of a Reichardt-Type Dye
3	Claudio Amovilli	Size-extensive wave functions for QMC: The J-LGVBn theory
4	Iva Angelova	Combined ab initio/semi-empirical Screening Protocol for Properties of Self-Assembled Monolayers
5	Luis Paulo Barbour Scott	Flexibility of Hunam Thioredoxin 1 and new biding sites using Normal Modes Analysis
6	Attila Bende	DNA - Protein interaction in the nucleosome system
7	Victor Bernstein	Impact induced multifragmentation of fullerene on gold: experimentally motivated molecular dynamics simulations
8	Debarati Bhattacharya	Formulation of partial triples to the electronic transition dipole moments within Fock-space multi-reference coupled cluster framework
9	Kim Bolton	Molecular-level simulations of permeation in polymer films and fibres
10	Lukas Bucinsky	Spin at the 2-component level of theory. The way in pain
11	Adem Cinarli	Theoretical DFT, FT-IR and NMR studies of 2-methoxy-6-(5-F/Cl/Br-1H-benzimidazol-2-yl)-phenols
12	Kota Daigoku	Visualization and characterization of intermolecular interaction based on the electron difference density
13	Justyna Dominikowska	Halogen-halogen interaction in light of many-body approach.
14	Matus Dubecky	Noncovalent Interactions: Quantum Monte Carlo Approaches CCSD(T) to 0.1 kcal/mol
15	Janus Eriksen	A novel framework for deriving triples and quadruples corrections to the CCSD energy
16	Olle Falklöf	Modeling of Phytochrome Absorption Spectra
17	Attila Fekete	The proteolytic reaction of papain: ONIOM-type hybrid QM/MM calculations and Poisson-Boltzmann electrostatic correction

Papers in Poster Session I cont'd

No.	Name	Title
18	Franca Maria Floris	A Polarizable Continuum Model of solvation designed for QMC: ground and excited states of solutes
19	Jerome Gomar	A combined experimental and theoretical study on the structure of genipin in solution
20	Jaroslav Granatier	The quartet-quartet crossing in Ir...benzene half-sandwich complex
21	Demet Gürbüz	Theoretical and spectral characterization of 5,6-dichloro-2-(2′,3′/2′,4′/2′,5′/3′,4′/3′,5′-dimethoxyphenyl)-1H-benzimidazoles
22	Merouani Hafida	DFT Study of the Stereo-Selectivity of Oxygenated Heterocycles from 10 to 12 Links
23	Matti Hellström	Cu on ZnO: alternating Cu charge states and accurate adsorption energy calculations upon charge transfer
24	Robert Izsak	The Equation of Motion Coupled Cluster Approach as Implemented in ORCA
25	Tomasz Janowski	Natural Correlation Orbitals in Local Laplace Transformed Triples (T) Correction
26	Hyunjun Ji	Convergence Acceleration of Relaxation-Separated Many-Body Expansion for Periodic Systems
27	Sayali Joshi	Calculation of response properties using Extended Coupled Cluster Method
28	Apostolos Kalemos	Symmetry breaking in a nutshell. The odyssey of a pseudo problem in molecular physics. The X BNB case revisited.
29	Uraiwan Kamolphop	A density functional investigation of ethylene adsorption on graphene surfaces
30	Frantisek Karlicky	Non-covalent Interactions to Graphene: Theory and Experiment
31	Małgorzata Kauch	Metal-substituted rubredoxin – theoretical prediction of the spin spin coupling constants using ZORA
32	Ali Kazemi Babhydari	Characterization of protein-ligand complexes using molecular dynamics simulations by consideration of GABAA protein as receptor and Lavender compounds as ligand
33	Maria Khrenova	Proteolysis mechanism in matrix metalloproteinases suggested by molecular modeling
34	Jaehoon Kim	A simple and accurate non-emperical doubly-hybrid density functional using quadratic approximation of adiabatic connection formula
35	Yukiumi Kita	Theoretical investigation of the binding of a positron to vibrational excited states of hydrogen cyanide molecule
36	Malte Kokoschka	Methods for the accurate description of Platinum-DNA interaction
37	Christoph Köppl	Automated optimisation of quantum chemical algorithms within an integrated tensor framework

Papers in Poster Session I cont'd

No.	Name	Title
38	Takako Kudo	Ab Initio Molecular Dynamics Simulations of H_2 Formation inside POSS Compounds
39	Antonio Largo	Theoretical studies of possible routes for the synthesis of amino acids in space
40	Tian Lu	Integrating the Laplacian of electron density in fuzzy overlap space as a measure of covalent bond order
41	Alejandro Fabián Maldonado	Relativistic and correlation effects on heavy molecules containing Sn and Pb atoms
42	Bhabani Mallik	Structure and Dynamics of ionic liquids from first principles simulations: Effects of dispersion corrected density functionals and charge density cutoff
43	Aya Matsuda	Electronic structures and hydrogen absorption properties of Pd/Pt clusters : What is the difference from bulk?
44	Yu-ichiro Matsushita	Microscopic mechanism of band-gap variations in SiC polytypes based on ab initio calculations: Roles of peculiar electron state floating in internal space
45	Petr Milko	Electronic Structure of Iron Complexes Containing Bipyridine-based PNN Pincer Ligands
46	Noriyuki Mizoguchi	Edge Effect in Finite-length Pentaheptite Nanotubes
47	Alena Moon	Solvation of tert-Butyl Alcohol in Water: An Effective Fragment Potential Study
48	Hirotoshi Mori	Electronic Band Structure Calculations on Thin Films of the $L2_1$ Full Heusler Alloys X_2YSi (X, Y = Mn, Fe, and Co): toward Spintronic Materials
49	Bastien Mussard	Analytical gradients of Random Phase Approximation correlation energies in Range-Separated-Hybrid context: theory and implementation
50	Péter Nagy	Optical activity spectra of carbon nanostructures via a novel pi-electron model
51	Szilvia Nagy	Adaptive refinement of wavelet based solutions of the Schrödinger equation by independent estimation of the fine resolution coefficients
52	Katsumi Nakagawa	Structure Optimization of Molecules Consisting of up to Period 5 Elements by Discrete Variational Xalpha Method
53	Michaela Nekardova	Quantum chemical study of binding affinity of the purine inhibitor and its bioisosteres to cyclin-dependent kinases
54	Anton Nizovtsev	Electronic rearrangements during the inversion of lead phthalocyanine
55	Nadtanet Nunthaboot	Comparison of the monomer structure of the FMN binding protein from Desulfovibrio vulgaris obtained by NMR and molecular dynamics simulation approaches
56	Miho Otsuka	Theoretical Study on Internal Alkyne/Vinylidene Isomerization on Group 8 Transition Metal Complexes

Papers in Poster Session I cont'd

No.	Name	Title
57	Ivana Paidarova	Chemistry of defects in solids
58	Balazs Pinter	Structural and Electronic Contributions to Redox-noninnocent Behavior
59	Philipp Nikolaus Pleßow	Carbon-Carbon bond activation of epoxides by a (dtbpm)Pt fragment – A theoretical study.
60	Zoltán Rolik	Towards a multireference coupled-cluster method based on a unitary transformation
61	Thanyada Rungrotmongkol	Binding mode and binding affinity prediction of inclusion complex between flavonoid and ß-cyclodextrin
62	Pradipta Kumar Samanta	Formulation of an Internally Contracted Multi-Reference Coupled-Cluster Based Linear Response Theory to Study Excited States
63	Carlos Silva	Structure- and Ligand-based Drug Design of Novel p38 Alpha MAPK Inhibitors in the Fight Against the Alzheimer's Disease.
64	Gabriella Skara	Probe molecule transformations for staining techniques in zeolites – A periodic DFT study
65	Victor Solomonik	Jahn–Teller, pseudo-Jahn–Teller, and spin-orbit coupling effects in cerium trihalide molecules
66	Elizaveta Suturina	The quantum chemical study of isotropic and anisotropic magnetic properties of molecular magnets
67	Péter Szabó	Isomerization effect on the dynamics of the H + O2 collision
68	Lóránt Szegedy	An efficient linear-scaling CCSD(T) method based on local natural orbitals
69	Luca Szegletes	Parallel Evaluation of Two-Electron Integrals using a Wavelet Approach on the Graphics Processor Unit
70	Keiko Takano	A theoretical study of the interaction between a lectin called Siglec-7 and its glycan ligand in the immune system
71	Aydin Tavman	Theoretical DFT, FT-IR and NMR studies of 2-methoxy-6-(5-H/Me/NO2-1H-benzimidazol-2-yl)-phenols
72	Zsuzsanna Tóth	Approximate lower bounds via Löwdin's bracketing function
73	Yuzuru Ujiie	Molecular dynamics study on the substrate binding free energy of Threonine Synthase
74	Nikita Vakula	Theoretical investigations of Ag/SiO_2 interface
75	Marta Wiśniewska	Potential of mean force of association of hydrophobic particles: dependence on size and temperature
76	Nurbosyn U. Zhanpeisov	Modified new carbon K4 and metal-organic framework structures: A theoretical DFT study
77	Tamás Zoboki	Linearized Coupled Cluster Corrections to Antisymmetrized Product of Strongly Orthogonal Geminals: role of dispersive interactions

Papers in Poster Session II

No.	Name	Title
1	Tomoko Akama	Real-time TDHF/TDDFT calculation with efficient time evolution
2	Zikri Altun	Modeling Spin Crossover Complexes
3	Koji Ando	Electron Transfer Pathway in Biomolecules: FMO-LCMO and Tunneling Pathway Analysis
4	Arifin	Theoretical Study of Glucose Transformation to 5-Hydroxymethylfurfural using RISM-SCF-SEDD
5	Bence Babinszki	The hydrolysis of alpha-iminocarbonyls – a quantum chemical mechanistic study
6	Carmen Barrientos	Reactivity of first-row transition metal monocations with methyl fluoride: a computational kinetic study
7	Hamid Berriche	Structure and Spectra modeling of CsRg (Rg=Ar, Xe, Kr) van der Waals Complexes
8	Edward Brothers	Limitations of reaction barrier benchmarks with fixed geometries
9		cancelled
10	Francesca Costanzo	Hydrogen dissociation on aluminum cluster interacting with carbon surfaces by first principles calculations
11	András Csehi	Theoretical investigation of molecular switch properties of several quinoline compounds
12	Botond Csontos	Dissociation of the fluorine molecule: A benchmark study
13	Jozsef Csontos	Analytic gradients for general non-iterative coupled-cluster approaches
14	Malgorzata Domagala	The substituent effect in the doubly-charged benzene
15	Faina Dubnikova	Products of quinoline thermal decomposition and theirs further reactions. Quantum chemical calculations and kinetic modeling
16	Patrick Ettenhuber	Integral direct and memory conservative CCSD algorithm
17	Felipe Fantuzzi	Revisiting the aromaticity concept: electrostatic effects are responsible for the stability of benzene towards ring distortions
18	Nicolas Fernandez	Is DFT reliable for beryllium containing systems? The example of the Be – π system interaction

Papers in Poster Session II cont'd

No.	Name	Title
19	Leon Freitag	A new look at the electronic structure of the $\{RuNO\}^6$ moiety using density-fitting CASSCF calculations and localised orbitals
20	Werner Gyorffy	Analytical energy gradients for explicitly correlated second-order Moller-Plesset perturbation theory
21	Susanta Haldar	On the Association of the Base Pairs on the Silica Surface Based on Free Energy Biased Molecular Dynamics Simulation and Quantum Mechanical Calculations
22	Stefan Huber	Stabilization mechanisms at polar ZnO surfaces in ideal vacuum conditions: a SCC-DFTB study
23	Yasuhiro Ikabata	Local response dispersion method in periodic systems: Implementation in the package based on a plane-wave basis set
24	Rodica-Mariana Ion	CNDO/2 and Tamm-Dancoff methods for electronic structure evaluation of aluminum porphyrins involved in photodynamic therapy
25	Munendra Jain	Theoretical Study of Protein Flexibility During Molecular Docking
26	Nopporn Kaiyawet	Theoretical study on ternary complex stability and Michael addition reactivity of Thymidylate synthase/mTHF/XdUMP
27	Ilya Kaliman	Reusable software for quantum chemistry applications
28	Emile Kassab	Theoretical Study of the Dispersive Interactions Effects on the Adsorption properties of 4,4'-Bipyridine in H-ZSM-5 Zeolite
29	Michio Katouda	Development of MPI/OpenMP hybrid parallel algorithm of resolution of identity second-order Møller–Plesset perturbation calculations for massively parallel multicore supercomputers
30	Toshiaki Kawamura	Quantum-Chemical Calculations of 195Pt-NMR Chemical Shifts in Platinum(IV) Porphyrins with Axial Ligands (Cl- , Br- , I- , SCN-)
31	Andrew King	The effect of non-linear variational parameters on the energy convergence of Coulomb three-body systems
32	Steven Kirk	AIMPAC2: A next-generation QTAIM code
33	Jiri Klimes	Acceleration of basis set convergence of ACFDT-RPA and MP2 correlation energies using effective energy techniques
34	István Komáromi	The Early Phase of the Conformational Transition at Vertebrate Transglutaminases; Can We See it From Molecular Dynamics Simulations?
35	Piotr Kowalski	Predicting excitation energies from short-range density functionals combined with the long-range strongly orthogonal geminal theory
36	Justyna Kozłowska	Electric-dipole properties of spatially confined water molecule
37	Kasper Kristensen	The Divide-Expand-Consolidate MP2 scheme goes massively parallel

Papers in Poster Session II cont'd

No.	Name	Title
38	Noriyuki Kurita	Specific interactions between lactose repressor protein and DNA: classical MD and ab initio MO calculations
39	Michal Malček	Comparison between the contact and effective electron/spin densities at the IOTC quasirelativistic level of theory
40	Marco Masia	On the Excitation Energy Transfer Dependency on Pigment–Protein Interactions in the Fenna–Matthews–Olsen Complex.
41	Toru Matsui	A Density Functional Theory Based Protocol to Compute the Redox Potential for Transition Metal Complexes
42	Arthitaya Meeprasert	Classical and advanced molecular dynamics study on ligand-protein interactions targeted at HCV NS3/4A protease
43	Vladimir Mironov	Photoswitching of the kindiling fluorescent protein: a theoretical study
44	Wataru Mizukami	A second-order multi-reference perturbation method for molecular vibrations
45	Dmitry Morozov	Probing the effect of the environment on the excited state dynamics of biological chromophores by ab initio quantum chemistry.
46	Salvador Moncho Escriva	Performance of Density Functionals in Modeling the Decomposition of CH_3OH by Cu_4 Cluster
47	Yutaka Nakatsuka	Development of Relativistic Quantum Monte Carlo: Theory and parallel program
48	Sébastien Nénon	Origin of the surface-induced first hyperpolarizability in the C_{60}/SiO_2 system: a SCC-DFTB insight.
49	Yoshio Nishimoto	Theoretical and Experimental Investigations of an Aldol-type Reaction with Rh Complex
50	Kaori Noto	Fragment molecular orbital and MD calculation study: Interaction analysis of HIV-1 antibody 2G12 and glycan Ligand
51	Hiroki Otaki	Acceleration of the vibrational structure calculation with optimized vibrational coordinates
52	Takao Otsuka	Theoretical study of DNA with unnatural base pair system using order-N DFT calculations
53	Nadia Ouddai	Theoretical Investigation of Ytterbium Tri-chelates Compounds
54	Abdelhamid Ounissi	The Nature of the Metal-acetylide Interaction in the Ternary Transition Metal Acetylide Complex $C_5Me_5Ti[\eta\text{-}C_2(SnMe_3)_2]$
55	Deepa Palanisamy	Quantum Chemistry-based Docking and Scoring for Design of Protein Kinase Inhibitors
56	Marcin Palusiak	Studies on halogen bonding
57	Ewa Pastorczak	Employing ensemble variational principle to calculate electron excitation energies of molecules: a range-separated approach

Papers in Poster Session II cont'd

No.	Name	Title
58	José Juan Peña	Exactly-solvable position-dependent mass Schrödinger equation for the Thomas-Fermi and Harmonic Oscillator potentials.
59	Jiri Pittner	Fluorescence of PRODAN in Water: a Computational QM/MM MD Study
60	Malinee Promkatkaew	Photophysical Properties and Photochemistry of Substituted Cinnamates for UVB Blocking: Effect of Hydroxy, Nitro, and Fluoro Substitutions at ortho, meta, and para Positions
61	Peter Reinhardt	Dispersion-only approximation for long-range RPA correlation contributions to DFT intermolecular interaction energies
62	Julia Romanova	Vibronic and Resonance Raman Spectra of Extended Viologens Modelled by Multireference Approaches
63	Agnieszka Roztoczyńska	Two-photon absorption spectra of the spiropyran and merocyanine pair: A comparative study of solvation models
64	Lakehal Salima	Theoretical Investigation on Homoleptic Yttrium Triguanidinates:
65	Benjamin Sanchez Lengeling	A Quantum Monte Carlo and CIPSI case study: Magnetic Coupling of a meta-xylylene diradical.
66	Mitsuo Shoji	Theoretical investigation on the absorption spectrum of photosystem as a biomarker on extrasolar planets
67	Raman Singh	Reaction Energetics of the Diels-Alder Reactions: A Long-range Corrected Density Functional Theory Study
68	Jan Šmydke	Generalization of the Non-Redundant Fockian for $N > 2$ electronic systems: Application to Excited States of Be Atom
69	Victor Solomonik	Towards accurate ab initio thermochemistry and spectroscopy of lanthanide compounds: Quantifying basis set, electron correlation, and spin-orbit coupling effects in lanthanide species
70	José Surga	Atomistic Study of the Incorporation Effect of Guest Ions Mg^{2+}, Al^{3+} and Fe^{3+} in Crystalline Structure Models of Cementitious Phases Like Alite (C_3S) and Belite (C_2S)
71	Milán Szőri	Cheap HEAT protocol: CHEAT1
72	Wataru Tanaka	Theoretical research on the substrate specificity of uridine-cytidine kinase
73	Tiago Teodoro	Prolapse-Free Relativistic Adapted Gaussian Basis Sets for 87Fr up to 118Uuo
74	Carl Trindle	Computational Thermochemistry of Superbases Derived from the Cyclopropene Imine Core
75	Kosuke Usui	Theoretical investigation of the electron transfer process in water
76	Anna Vnuchenko	Determine damage depth profiling by high-energy ion channeling in Monocrystalls
77	Takeshi Yoshikawa	Acceleration of divide-and-conquer method on GPU

List of Contributors

Family name	Given Name	Scheduled on				
Addicoat	Matthew	Monday	Evening		Aula	18 : 00
Akama	Tomoko	Thursday	Evening		Aula	18 : 00
Allen	Wesley	Thursday	Afternoon		Brahms	15 : 00
Allolio	Christoph	Monday	Evening		Aula	18 : 00
Altun	Zikri	Thursday	Evening		Aula	18 : 00
Amovilli	Claudio	Monday	Evening		Aula	18 : 00
Ando	Koji	Thursday	Afternoon	II	Bartók	17 : 40
Ando	Koji	Thursday	Evening		Aula	18 : 00
Angelova	Iva	Monday	Evening		Aula	18 : 00
Angyan	Janos	Friday	Morning	I	Bartók	8 : 30
Arifin		Thursday	Evening		Aula	18 : 00
Ayers	Paul	Wednesday	Morning	II	Pátria	11 : 30
Babinszki	Bence	Thursday	Evening		Aula	18 : 00
Barbour Scott	Luis Paulo	Monday	Evening		Aula	18 : 00
Barrientos	Carmen	Thursday	Evening		Aula	18 : 00
Bartlett	Rodney	Thursday	Morning	I	Bartók	8 : 30
Basilevsky	Mikhail	Thursday	Afternoon		Brahms	15 : 30
Becke	Axel	Tuesday	Morning	I	Bartók	9 : 00
Bende	Attila	Monday	Evening		Aula	18 : 00
Bende	Attila	Thursday	Afternoon		Brahms	14 : 30
Bernstein	Victor	Monday	Evening		Aula	18 : 00
Berriche	Hamid	Thursday	Evening		Aula	18 : 00
Bhattacharya	Debarati	Monday	Evening		Aula	18 : 00
Bhatt	Jayesh	Thursday	Afternoon	I	Lehár	15 : 00
Bil	Andrzej	Thursday	Morning	I	Lehár	10 : 10
Bolton	Kim	Monday	Evening		Aula	18 : 00
Brändas	Erkki	Wednesday	Morning	II	Bartók	11 : 00
Broer	Ria	Monday	Afternoon	I	Pátria	15 : 30
Brothers	Edward	Thursday	Evening		Aula	18 : 00
Bucinsky	Lukas	Monday	Evening		Aula	18 : 00
Cailliez	Fabien	Tuesday	Afternoon	I	Brahms	15 : 30
Cammi	Roberto	Monday	Afternoon	I	Lehár	16 : 00
Carsky	Petr	Monday	Morning	II	Lehár	11 : 00

List of Contributors cont'd

Family name	Given Name	Scheduled on				
Castro	Miguel	Friday	Afternoon	I	Bartók	15 : 30
Chai	Jeng-Da	Tuesday	Morning	II	Bartók	12 : 10
Champagne	Benoit	Tuesday	Morning	I	Lehár	10 : 10
Chen	Feiwu	Monday	Morning	II	Lehár	11 : 50
Cheng	Lan	Monday	Morning	II	Pátria	12 : 00
Cinarli	Adem	Monday	Evening		Aula	18 : 00
Costanzo	Francesca	Thursday	Evening		Aula	18 : 00
Cox	Hazel	Wednesday	Afternoon		Bartók	15 : 00
Crawford	Daniel	Friday	Afternoon	I	Pátria	15 : 30
Cremer	Dieter	Monday	Morning	II	Pátria	11 : 30
Csehi	András	Thursday	Evening		Aula	18 : 00
Csontos	Botond	Thursday	Evening		Aula	18 : 00
Csontos	Jozsef	Thursday	Evening		Aula	18 : 00
Cui	Qiang	Monday	Morning	II	Bartók	11 : 00
Daigoku	Kota	Monday	Evening		Aula	18 : 00
Daru	Janos	Thursday	Afternoon	II	Lehár	17 : 20
de Wergifosse	Marc	Monday	Afternoon	I	Bartók	15 : 20
Dobson	John	Friday	Morning	II	Bartók	11 : 30
Doltsinis	Nikos	Thursday	Afternoon	II	Lehár	16 : 30
Domagala	Malgorzata	Thursday	Evening		Aula	18 : 00
Dominikowska	Justyna	Monday	Evening		Aula	18 : 00
Dopieralski	Przemyslaw	Thursday	Morning	II	Lehár	11 : 30
Draxl	Claudia	Tuesday	Morning	I	Lehár	9 : 00
Dubecky	Matus	Monday	Evening		Aula	18 : 00
Dubnikova	Faina	Thursday	Evening		Aula	18 : 00
Efremenko	Irena	Wednesday	Morning	I	Lehár	10 : 10
El-Azhary	Adel	Thursday	Morning	I	Brahms	8 : 50
Engin	Selma	Wednesday	Morning	I	Lehár	9 : 30
Ensing	Bernd	Thursday	Morning	I	Lehár	9 : 10
Eriksen	Janus	Monday	Evening		Aula	18 : 00
Ernzerhof	Matthias	Friday	Afternoon	I	Bartók	15 : 00
Ettenhuber	Patrick	Thursday	Evening		Aula	18 : 00
Falklöf	Olle	Monday	Evening		Aula	18 : 00
Fantuzzi	Felipe	Thursday	Evening		Aula	18 : 00
Fdez. Sanz	Javier	Tuesday	Afternoon	I	Lehár	16 : 10
Fekete	Attila	Monday	Evening		Aula	18 : 00
Fernandez	Nicolas	Thursday	Evening		Aula	18 : 00
Filatov	Michael	Wednesday	Morning	II	Bartók	11 : 50

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Family name	Given Name	Scheduled on				
Fink	Reinhold	Thursday	Morning	I	Bartók	9 : 50
Floris	Franca Maria	Monday	Evening		Aula	18 : 00
Freitag	Leon	Thursday	Evening		Aula	18 : 00
Frenking	Gernot	Tuesday	Afternoon	I	Bartók	14 : 30
Frenklach	Michael	Tuesday	Morning	I	Brahms	9 : 00
Friedrich	Joachim	Friday	Morning	I	Pátria	10 : 10
Fromager	Emmanuel	Friday	Morning	I	Bartók	9 : 30
Furtenbacher	Tibor	Tuesday	Morning	II	Brahms	12 : 10
Gadre	Shridhar	Friday	Morning	II	Pátria	11 : 30
Geerlings	Paul	Tuesday	Afternoon	II	Bartók	18 : 30
Ghysels	An	Tuesday	Morning	I	Lehár	9 : 30
Gill	Peter	Tuesday	Morning	I	Bartók	8 : 30
Gokhberg	Kirill	Monday	Afternoon	I	Lehár	15 : 00
Gomar	Jerome	Monday	Evening		Aula	18 : 00
Goos	Elke	Tuesday	Morning	II	Brahms	11 : 50
Góra	Robert	Wednesday	Morning	I	Lehár	9 : 50
Granatier	Jaroslav	Monday	Evening		Aula	18 : 00
Gromov	Evgeniy	Wednesday	Morning	I	Lehár	8 : 50
Gürbüz	Demet	Monday	Evening		Aula	18 : 00
Gyorffy	Werner	Thursday	Evening		Aula	18 : 00
Hafida	Merouani	Monday	Evening		Aula	18 : 00
Haldar	Susanta	Thursday	Evening		Aula	18 : 00
Halet	Jean-Francois	Tuesday	Afternoon	I	Lehár	14 : 30
Hanrath	Michael	Friday	Afternoon	I	Pátria	15 : 00
Hedegård	Erik Donovan	Monday	Morning	II	Bartók	11 : 50
Helgaker	Trygve	Wednesday	Morning	II	Pátria	12 : 00
Hellström	Matti	Monday	Evening		Aula	18 : 00
Hermansson	Kersti	Thursday	Morning	I	Lehár	8 : 30
Hermansson	Kersti	Tuesday	Morning	II	Lehár	11 : 30
Hirata	So	Friday	Morning	I	Pátria	8 : 50
Hobza	Pavel	Friday	Afternoon	II	Pátria	17 : 00
Hoffmann	Mark	Thursday	Morning	II	Bartók	11 : 00
Hoggan	Philip	Tuesday	Afternoon	II	Lehár	17 : 30
Høyvik	Ida-Marie	Friday	Morning	I	Pátria	9 : 50
Huber	Stefan	Thursday	Evening		Aula	18 : 00
Ikabata	Yasuhiro	Thursday	Evening		Aula	18 : 00
Ion	Rodica-Mariana	Thursday	Evening		Aula	18 : 00
Islam	Mazharul M.	Tuesday	Morning	II	Lehár	12 : 10
Izsak	Robert	Monday	Evening		Aula	18 : 00

List of Contributors cont'd

Family name	Given Name	Scheduled on				
Jain	Munendra	Thursday	Evening		Aula	18 : 00
Jankowski	Karol	Thursday	Morning	I	Bartók	9 : 30
Janowski	Tomasz	Monday	Evening		Aula	18 : 00
Jansen	Georg	Friday	Morning	I	Bartók	9 : 00
Jenkins	Samantha	Friday	Afternoon	I	Pátria	14 : 30
Jensen	Jan Halborg	Monday	Morning	I	Bartók	10 : 00
Jeszenszki	Péter	Tuesday	Afternoon	I	Brahms	16 : 10
Jeziorski	Bogumil	Friday	Morning	II	Bartók	11 : 00
Ji	Hyunjun	Monday	Evening		Aula	18 : 00
Joergensen	Poul	Wednesday	Morning	I	Pátria	8 : 40
Joshi	Sayali	Monday	Evening		Aula	18 : 00
Kaiyawet	Nopporn	Thursday	Evening		Aula	18 : 00
Kalemos	Apostolos	Monday	Evening		Aula	18 : 00
Kaliman	Ilya	Thursday	Evening		Aula	18 : 00
Kállay	Mihály	Wednesday	Morning	I	Pátria	8 : 30
Kamolphop	Uraiwan	Monday	Evening		Aula	18 : 00
Kapralova	Petra Ruth	Wednesday	Afternoon		Lehár	15 : 40
Karadakov	Peter	Tuesday	Afternoon	I	Bartók	15 : 50
Karlicky	Frantisek	Monday	Evening		Aula	18 : 00
Karlicky	Frantisek	Tuesday	Afternoon	I	Lehár	15 : 50
Kassab	Emile	Thursday	Evening		Aula	18 : 00
Katouda	Michio	Thursday	Evening		Aula	18 : 00
Kauch	Małgorzata	Monday	Evening		Aula	18 : 00
Kauczor	Joanna	Wednesday	Morning	I	Lehár	9 : 10
Kawamura	Toshiaki	Thursday	Evening		Aula	18 : 00
Kazemi Babhydari	Ali	Monday	Evening		Aula	18 : 00
Kertesz	Miklos	Tuesday	Afternoon	I	Lehár	15 : 00
Khrenova	Maria	Monday	Evening		Aula	18 : 00
Kim	Jaehoon	Monday	Evening		Aula	18 : 00
King	Andrew	Thursday	Evening		Aula	18 : 00
Kirk	Steven	Thursday	Evening		Aula	18 : 00
Kiselev	Vitaly	Thursday	Morning	I	Brahms	9 : 30
Kita	Yukiumi	Monday	Evening		Aula	18 : 00
Klimes	Jiri	Thursday	Evening		Aula	18 : 00
Kobayashi	Masato	Thursday	Afternoon	II	Bartók	17 : 00
Kokoschka	Malte	Monday	Evening		Aula	18 : 00
Komáromi	István	Thursday	Evening		Aula	18 : 00
Köppl	Christoph	Monday	Evening		Aula	18 : 00
Kowalski	Piotr	Thursday	Evening		Aula	18 : 00
Kozłowska	Justyna	Thursday	Evening		Aula	18 : 00

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Family name	Given Name	Scheduled on				
Kraft	Markus	Tuesday	Afternoon	I	Brahms	15 : 00
Kraka	Elfi	Tuesday	Morning	II	Bartók	11 : 30
Kristensen	Kasper	Thursday	Evening		Aula	18 : 00
Krylov	Anna	Wednesday	Morning	I	Pátria	10 : 10
Kudo	Takako	Monday	Evening		Aula	18 : 00
Kurita	Noriyuki	Thursday	Evening		Aula	18 : 00
Kürti	Jenő	Tuesday	Afternoon	II	Lehár	18 : 00
Kutzelnigg	Werner	Monday	Morning	I	Pátria	10 : 00
Largo	Antonio	Monday	Evening		Aula	18 : 00
Legeza	Ors	Monday	Morning	II	Lehár	11 : 30
Lendvay	György	Monday	Afternoon	I	Lehár	14 : 30
Lindgren	Ingvar	Friday	Afternoon	II	Pátria	17 : 30
Li	Shuhua	Friday	Morning	I	Pátria	8 : 30
Liu	Wenjian	Monday	Morning	II	Pátria	11 : 00
Lu	Tian	Monday	Evening		Aula	18 : 00
Magyarfalvi	Gábor	Thursday	Morning	II	Brahms	12 : 10
Ma	Haibo	Thursday	Afternoon	II	Lehár	17 : 40
Ma	Jing	Monday	Afternoon	I	Lehár	15 : 20
Malček	Michal	Thursday	Evening		Aula	18 : 00
Maldonado	Alejandro Fabián	Monday	Evening		Aula	18 : 00
Mallik	Bhabani	Monday	Evening		Aula	18 : 00
Martyna	Glenn	Friday	Morning	I	Bartók	10 : 10
Marzari	Nicola	Tuesday	Morning	II	Lehár	11 : 00
Masia	Marco	Thursday	Evening		Aula	18 : 00
Masia	Marco	Thursday	Morning	I	Lehár	8 : 40
Matsuda	Aya	Monday	Evening		Aula	18 : 00
Matsui	Toru	Thursday	Evening		Aula	18 : 00
Matsushita	Yu-ichiro	Monday	Evening		Aula	18 : 00
Maurer	Reinhard	Tuesday	Afternoon	I	Lehár	15 : 30
Mayer	Istvan	Tuesday	Afternoon	II	Bartók	18 : 00
Mazumdar	Sumit	Tuesday	Morning	I	Lehár	8 : 30
Meeprasert	Arthitaya	Thursday	Evening		Aula	18 : 00
Mezey	Paul	Wednesday	Morning	II	Bartók	12 : 10
Michl	Josef	Friday	Afternoon	II	Pátria	16 : 30
Milko	Petr	Monday	Evening		Aula	18 : 00
Mironov	Vladimir	Thursday	Evening		Aula	18 : 00
Mitschker	Jan	Thursday	Morning	I	Brahms	9 : 50
Mizoguchi	Noriyuki	Monday	Evening		Aula	18 : 00

List of Contributors cont'd

Family name	Given Name	Scheduled on				
Mizukami	Wataru	Thursday	Evening		Aula	18 : 00
Moiseyev	Nimrod	Wednesday	Afternoon		Bartók	14 : 30
Moncho Escriva	Salvador	Thursday	Evening		Aula	18 : 00
Moon	Alena	Monday	Evening		Aula	18 : 00
Mori	Hirotoshi	Monday	Evening		Aula	18 : 00
Morozov	Dmitry	Thursday	Evening		Aula	18 : 00
Mukherjee	Debashis	Wednesday	Morning	I	Pátria	9 : 40
Musial	Monika	Monday	Morning	I	Lehár	10 : 10
Mussard	Bastien	Monday	Evening		Aula	18 : 00
Nagy	Ágnes	Friday	Afternoon	I	Bartók	14 : 30
Nagy	Péter	Monday	Evening		Aula	18 : 00
Nagy	Szilvia	Monday	Evening		Aula	18 : 00
Nakagawa	Katsumi	Monday	Evening		Aula	18 : 00
Nakai	Hiromi	Wednesday	Afternoon		Pátria	15 : 30
Nakano	Masayoshi	Thursday	Morning	II	Brahms	11 : 50
Nakatsuka	Yutaka	Thursday	Evening		Aula	18 : 00
Náray-Szabó	Gábor	Monday	Afternoon	I	Bartók	15 : 00
Nascimento	Marco	Tuesday	Afternoon	I	Bartók	15 : 30
Naumkin	Fedor	Wednesday	Afternoon		Lehár	15 : 20
Nebgen	Ben	Thursday	Afternoon	I	Lehár	15 : 20
Neese	Frank	Wednesday	Afternoon		Pátria	15 : 00
Nekardova	Michaela	Monday	Evening		Aula	18 : 00
Nemeth	Karoly	Tuesday	Morning	II	Lehár	11 : 50
Nemukhin	Alexander	Wednesday	Morning	II	Lehár	11 : 30
Nénon	Sébastien	Thursday	Evening		Aula	18 : 00
Nicolaides	Cleanthes	Wednesday	Morning	I	Bartók	8 : 30
Nishimoto	Yoshio	Thursday	Evening		Aula	18 : 00
Nizovtsev	Anton	Monday	Evening		Aula	18 : 00
Noga	Jozef	Thursday	Afternoon	II	Bartók	16 : 30
Nordlund	Kai	Thursday	Morning	II	Lehár	11 : 00
Noto	Kaori	Thursday	Evening		Aula	18 : 00
Nunthaboot	Nadtanet	Monday	Evening		Aula	18 : 00
Nyman	Gunnar	Thursday	Morning	I	Lehár	9 : 40
Ochsenfeld	Christian	Thursday	Morning	I	Bartók	9 : 00
Olivares-Amaya	Roberto	Thursday	Afternoon	II	Bartók	17 : 20
Olm	Carsten	Tuesday	Morning	II	Brahms	11 : 30
Olsen	Jeppe	Thursday	Afternoon	I	Bartók	14 : 30
Otaki	Hiroki	Thursday	Evening		Aula	18 : 00
Otsuka	Miho	Monday	Evening		Aula	18 : 00

List of Contributors cont'd

Family name	Given Name	Scheduled on				
Otsuka	Takao	Thursday	Evening		Aula	18 : 00
Ouddai	Nadia	Thursday	Evening		Aula	18 : 00
Ounissi	abdelhamid	Thursday	Evening		Aula	18 : 00
Paidarova	Ivana	Monday	Evening		Aula	18 : 00
Paidarova	Ivana	Wednesday	Morning	I	Bartók	10 : 00
Palanisamy	Deepa	Thursday	Evening		Aula	18 : 00
Palusiak	Marcin	Thursday	Evening		Aula	18 : 00
Pápai	Imre	Thursday	Morning	I	Brahms	9 : 10
Pastorczak	Ewa	Thursday	Evening		Aula	18 : 00
Pecul	Magdalena	Monday	Morning	II	Bartók	11 : 30
Peña	José Juan	Thursday	Evening		Aula	18 : 00
Pernal	Katarzyna	Thursday	Morning	II	Bartók	11 : 30
Piecuch	Piotr	Thursday	Afternoon	I	Bartók	15 : 30
Pierloot	Kristine	Tuesday	Morning	I	Bartók	9 : 30
Pinter	Balazs	Monday	Evening		Aula	18 : 00
Piris	Mario	Thursday	Morning	II	Bartók	12 : 10
Pittner	Jiri	Thursday	Evening		Aula	18 : 00
Pittner	Jiri	Thursday	Morning	II	Bartók	11 : 50
Pleßow	Philipp Nikolaus	Monday	Evening		Aula	18 : 00
Podeszwa	Rafal	Friday	Morning	I	Bartók	9 : 50
Prezhdo	Oleg	Wednesday	Morning	II	Lehár	12 : 00
Promkatkaew	Malinee	Thursday	Evening		Aula	18 : 00
Pulay	Peter	Monday	Afternoon		Pátria	16 : 50
Pyykkö	Pekka	Monday	Afternoon	I	Pátria	14 : 30
Rassolov	Vitaly	Thursday	Afternoon	I	Bartók	15 : 00
Reinhardt	Peter	Thursday	Evening		Aula	18 : 00
Rolik	Zoltán	Monday	Evening		Aula	18 : 00
Romanova	Julia	Thursday	Evening		Aula	18 : 00
Romera	Elvira	Monday	Morning	II	Lehár	12 : 10
Rosta	Edina	Monday	Morning	II	Bartók	12 : 10
Roztoczyńska	Agnieszka	Thursday	Evening		Aula	18 : 00
Rungrotmongkol	Thanyada	Monday	Evening		Aula	18 : 00
Rupnik	Kresimir	Monday	Afternoon	I	Bartók	16 : 00
Ruscic	Branko	Tuesday	Afternoon	I	Brahms	14 : 30
Ruud	Kenneth	Monday	Afternoon	I	Lehár	15 : 40
Saalfrank	Peter	Wednesday	Morning	II	Bartók	11 : 30
Salahub	Dennis	Monday	Afternoon	I	Bartók	14 : 30
Salima	Lakehal	Thursday	Evening		Aula	18 : 00

List of Contributors cont'd

Family name	Given Name	Scheduled on				
Salvador	Pedro	Wednesday	Afternoon		Lehár	14 : 30
Samanta	Pradipta Kumar	Monday	Evening		Aula	18 : 00
Sanchez Lengeling	Benjamin	Thursday	Evening		Aula	18 : 00
Saue	Trond	Monday	Afternoon	I	Pátria	15 : 00
Savin	Andreas	Tuesday	Afternoon	I	Bartók	15 : 00
Schuetz	Martin	Friday	Morning	I	Pátria	9 : 20
Scrinzi	Armin	Wednesday	Morning	I	Bartók	9 : 30
Scuseria	Gustavo	Monday	Morning	I	Pátria	8 : 30
Shapiro	Moshe	Wednesday	Morning	I	Bartók	9 : 00
Sheen	David	Tuesday	Morning	II	Brahms	11 : 00
Sheka	Elena	Wednesday	Morning	I	Lehár	8 : 30
Shigeta	Yasuteru	Thursday	Morning	II	Brahms	11 : 30
Shoji	Mitsuo	Thursday	Evening		Aula	18 : 00
Shurki	Avital	Tuesday	Morning	II	Bartók	11 : 50
Siegbahn	Per	Wednesday	Morning	II	Lehár	11 : 00
Silva	Carlos	Monday	Evening		Aula	18 : 00
Silverstone	Harris	Wednesday	Afternoon		Bartók	15 : 20
Singh	Raman	Thursday	Evening		Aula	18 : 00
Siuda	Paweł Artur	Thursday	Morning	II	Lehár	11 : 50
Skara	Gabriella	Monday	Evening		Aula	18 : 00
Slipchenko	Lyudmila	Monday	Morning	I	Bartók	9 : 30
Smiechowski	Maciej	Thursday	Afternoon	II	Lehár	17 : 00
Šmydke	Jan	Thursday	Evening		Aula	18 : 00
Sokalski	Andrzej	Monday	Afternoon	I	Bartók	15 : 40
Solomonik	Victor	Monday	Evening		Aula	18 : 00
Solomonik	Victor	Thursday	Evening		Aula	18 : 00
Spohr	Eckhard	Thursday	Afternoon	I	Lehár	14 : 30
Stanton	John	Wednesday	Afternoon		Pátria	14 : 30
Stoll	Hermann	Friday	Morning	II	Pátria	11 : 00
Stopkowicz	Stella	Monday	Morning	I	Pátria	9 : 30
Surga	José	Thursday	Evening		Aula	18 : 00
Suturina	Elizaveta	Monday	Evening		Aula	18 : 00
Szabó	Péter	Monday	Evening		Aula	18 : 00
Szalay	Péter	Wednesday	Morning	II	Pátria	11 : 00
Szegedy	Lóránt	Monday	Evening		Aula	18 : 00
Szegletes	Luca	Monday	Evening		Aula	18 : 00
Szőri	Milán	Thursday	Evening		Aula	18 : 00
Tachikawa	Masanori	Wednesday	Afternoon		Lehár	15 : 00
Tadjer	Alia	Thursday	Morning	I	Brahms	10 : 10

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Family name	Given Name	Scheduled on				
Tafipolski	Maxim	Thursday	Morning	II	Lehár	12 : 10
Takano	Keiko	Monday	Evening		Aula	18 : 00
Tamm	Toomas	Thursday	Morning	I	Brahms	8 : 30
Tanaka	Wataru	Thursday	Evening		Aula	18 : 00
Tavman	Aydin	Monday	Evening		Aula	18 : 00
Teodoro	Tiago	Thursday	Evening		Aula	18 : 00
Tkatchenko	Alexandre	Friday	Morning	II	Bartók	12 : 00
Tóth	Zsuzsanna	Monday	Evening		Aula	18 : 00
Trindle	Carl	Thursday	Evening		Aula	18 : 00
Tsuneda	Takao	Tuesday	Morning	I	Bartók	10 : 10
Turányi	Tamás	Tuesday	Morning	I	Brahms	8 : 30
Ugalde	Jesus	Tuesday	Afternoon	II	Bartók	17 : 00
Ujiie	Yuzuru	Monday	Evening		Aula	18 : 00
Urban	Miroslav	Tuesday	Morning	I	Lehár	9 : 50
Usui	Kosuke	Thursday	Evening		Aula	18 : 00
Vakula	Nikita	Monday	Evening		Aula	18 : 00
Varga	Tamas	Tuesday	Afternoon	I	Brahms	15 : 50
Vibók	Ágnes	Thursday	Morning	II	Brahms	11 : 00
Vnuchenko	Anna	Thursday	Evening		Aula	18 : 00
v. Szentpaly	Laszlo	Tuesday	Afternoon	II	Bartók	17 : 30
Wang	Hai	Tuesday	Morning	I	Brahms	10 : 00
Werner	Hans-Joachim	Wednesday	Morning	I	Pátria	9 : 10
Wiśniewska	Marta	Monday	Evening		Aula	18 : 00
Witek	Henryk	Wednesday	Afternoon		Bartók	15 : 40
Wodyński	Artur	Monday	Afternoon	I	Pátria	16 : 00
Yamazaki	Kaoru	Thursday	Afternoon	I	Lehár	15 : 40
Yang	Weitao	Tuesday	Morning	II	Bartók	11 : 00
Yoshikawa	Takeshi	Thursday	Evening		Aula	18 : 00
Yoshizawa	Kazunari	Tuesday	Afternoon	II	Lehár	17 : 00
Zádor	Judit	Tuesday	Morning	I	Brahms	9 : 30
Zgid	Dominika	Monday	Morning	I	Lehár	9 : 30
Zhanpeisov	Nurbosyn U.	Monday	Evening		Aula	18 : 00
Ziegler	Tom	Tuesday	Afternoon	I	Bartók	16 : 10
Zilberg	Shmuel	Tuesday	Morning	I	Bartók	9 : 50
Zoboki	Tamás	Monday	Evening		Aula	18 : 00

List of Participants

Given name	Family Name	Affiliation	Country
Matthew	Addicoat	Jacobs University Bremen	Germany
Tomoko	Akama	Sophia University	Japan
Wesley	Allen	University of Georgia	USA
Christoph	Allolio	MLU Halle	Germany
Zikri	Altun	Marmara University	Turkey
Claudio	Amovilli	University of Pisa, Department of Chemistry and Industrial Chemistry	Italy
Koji	Ando	Kyoto University	Japan
Iva	Angelova	BASF SE	Germany
Janos	Angyan	CNRS and Université de Lorraine	France
Arifin		Nagoya University	Japan
Paul	Ayers	McMaster University	Canada
Bence	Babinszki	Eotvos Lorand University	Hungary
Luis Paulo	Barbour Scott	UFABC-BRAZIL / ENS CACHAN	BRAZIL
Carmen	Barrientos	Universidad de Valladolid	Spain
Rodney	Bartlett	University of Florida	USA
Mikhail	Basilevsky	Photochemistry Center, Russian Academy of Sciences	Russian Federation
Axel	Becke	Dalhousie University	Canada
Attila	Bende	National Institute for Research and Development of Isotopic and Molecular Technologies	Romania
Victor	Bernstein	Technion - Israel Institute of Technology	Israel
Hamid	Berriche	King Khalid University	Saudi Arabia
Debarati	Bhattacharya	CSIR - National Chemical Laboratory (NCL)	India
Jayesh	Bhatt	University of Surrey	UK
Andrzej	Bil	Institute of Physical Chemistry, University of Zürich	Switzerland
Kim	Bolton	University of Boras	Sweden
Erkki	Brändas	Dept. Chemistry, Uppsala University	Sweden
Ria	Broer	University of Groningen	The Netherlands
Edward	Brothers	Texas A&M University at Qatar	Qatar

List of Participants cont'd

Given name	Family Name	Affiliation	Country
Lukas	Bucinsky	Slovak University of Technology	Slovakia
Fabien	Cailliez	Université Paris-Sud	France
Roberto	Cammi	University of Parma, Department of Chemistry	Italy
Petr	Carsky	J.Heyrovsky Institute of Physical Chemistry	Czech Republic
Miguel	Castro	Universidad Nacional Autonoma de Mexico	México
Jeng-Da	Chai	National Taiwan University	Taiwan
Benoit	Champagne	University of Namur	Belgium
Feiwu	Chen	University of Science and Technology Beijing	P. R. China
Lan	Cheng	Department of Chemistry and BioChemistry, University of Texas at Austin	United States of America
Adem	Cinarli	Istanbul University	Turkey
Francesca	Costanzo	Leiden Institue of Chemistry	Netherlands
Hazel	Cox	University of Sussex	UK
Daniel	Crawford	Virginia Tech	USA
Dieter	Cremer	Department of Chemistry, SMU	USA
András	Csehi	University of Debrecen	Hungary
Botond	Csontos	Department of Physical Chemistry and Materials Science, Budapest University of Technology and Economics.	Hungary
Jozsef	Csontos	Budapest University of Technology and Economics	Hungary
Qiang	Cui	UW-Madison	USA
Kota	Daigoku	Kitasato University	Japan
Janos	Daru	Eötvös Loránd University, Physical Chemistry Department	Hungary
Marc	de Wergifosse	Université de Namur	Belgium
John	Dobson	Griffith University	Australia
Nikos	Doltsinis	University of Münster	Germany
Malgorzata	Domagala	Department of Theoretical and Structural Chemistry, University of Lodz	Poland
Justyna	Dominikowska	Department of Theoretical and Structural Chemistry, University of Lodz	Poland
Przemyslaw	Dopieralski	Lehrstuhl für Theoretische Chemie, Ruhr–Universität Bochum	Germany
Claudia	Draxl	HU Berlin, Physics Department	Germany
Matus	Dubecky	Palacky University Olomouc	Czech Republic

List of Participants cont'd

Given name	Family Name	Affiliation	Country
Faina	Dubnikova	The Hebrew University of Jerusalem	Israel
Bo	Durbeej	Division of Computational Physics, Linkoeping University	Sweden
Irena	Efremenko	Weizmann Institute of Science	Israel
Adel	El-Azhary	King Saud University	Saudi Arabia
Selma	Engin	Laboratoire de Chimie Physique - Matière et Rayonnement	France
Bernd	Ensing	University of Amsterdam	Netherlands
Janus	Eriksen	Aarhus University	Denmark
Matthias	Ernzerhof	University of Montreal	Canada
Patrick	Ettenhuber	Aarhus University	Denmark
Olle	Falklöf	Linköping University	Sweden
Felipe	Fantuzzi	Universidade Federal do Rio de Janeiro	Brazil
Javier	Fdez. Sanz	University of Seville	Spain
Attila	Fekete	Clinical Research Center, Medical and Health Science Center, University of Debrecen	Hungary
Nicolas	Fernandez	Aix-Marseille University	France
Michael	Filatov	University of Bonn	Germany
Reinhold	Fink	Physical and Theoretical Chemistry, Tübingen	Germany
Franca Maria	Floris	University of Pisa, Department of Chemistry and Industrial Chemistry	Italy
Géza	Fogarasi	Institute of Chemistry Eotvos University, Budapest	Hungary
Leon	Freitag	Institute of Theoretical Chemistry, University of Vienna	Austria
Gernot	Frenking	Philipps-Universität Marburg	Germany
Michael	Frenklach	UC Berkeley	USA
Joachim	Friedrich	Institute for Chemistry	Germany
Emmanuel	Fromager	University of Strasbourg	France
Tibor	Furtenbacher	Eotvos University	Hungary
Shridhar	Gadre	IIT Kanpur	India
Jürgen	Gauss	Institut für Physikalische Chemie, Universität Mainz	Germany
Paul	Geerlings	Vrije Universiteit Brussel	Belgium
An	Ghysels	Center for Molecular Modeling, Ghent University	Belgium
Peter	Gill	Australian National University	Australia
Kirill	Gokhberg	Heidelberg University	Germany

List of Participants cont'd

Given name	Family Name	Affiliation	Country
Tomasz	Janowski	University of Arkansas	USA
Georg	Jansen	University Duisburg-Essen	Germany
Samantha	Jenkins	Hunan Normal University	China
Jan Halborg	Jensen	University of Copenhagen	Denmark
Péter	Jeszenszki	Eotvos Lorand University	Hungary
Bogumil	Jeziorski	Department of Chemistry, University of Warsaw	Poland
Hyunjun	Ji	KAIST	Republic of Korea
Poul	Joergensen	Aarhus University	Denmark
Sayali	Joshi	CSIR National Chemical Laboratory	India
Nopporn	Kaiyawet	Chulalongkorn University	Thailand
Apostolos	Kalemos	Department of Chemistry, University of Athens	Greece
Ilya	Kaliman	Purdue University	USA
Mihály	Kállay	Department of Physical Chemistry and Materials Science, Budapest University of Technology and Economics	Hungary
Uraiwan	Kamolphop	Department of Chemistry, Faculty of Science, Mahasarakham University	Thailand
Petra Ruth	Kapralova	J. Heyrovsky Institute of Physical Chemistry, The Academy of Sciences of the Czech Republic	Czech Republic
Peter	Karadakov	University of York	UK
Frantisek	Karlicky	Palacky University Olomouc	Czech Republic
Emile	Kassab	CNRS	France
Michio	Katouda	RIKEN Advanced Institute for Computational Science	Japan
Małgorzata	Kauch	Faculty of Chemistry, University of Warsaw	Poland
Joanna	Kauczor	Linköping University	Sweden
Toshiaki	Kawamura	Tokyo Metropolitan University	Japan
Ali	Kazemi Babhydari	Department of Physical Chemistry, Islamic Azad University	Iran
Miklos	Kertesz	Georgetown University	USA
Maria	Khrenova	.N.Bach Institute of Biochemistry, Russian Academy of Sciences	Russia
Jaehoon	Kim	KAIST	Republic of Korea
Andrew	King	University of Sussex	England
Steven	Kirk	Hunan Normal University	China
Vitaly	Kiselev	Institute of Chemical Kinetics and Combustion SB RAS	Russia
Yukiumi	Kita	Yokohama City University	Japan

List of Participants cont'd

Given name	Family Name	Affiliation	Country
Jiri	Klimes	Faculty of Physics, University of Vienna	Austria
Masato	Kobayashi	Waseda University	Japan
Malte	Kokoschka	Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic	Czech Republic
István	Komáromi	Clinical Research Center, Medical & Health Science Center, University of Debrecen	Hungary
Christoph	Köppl	Institute of Theoretical Chemistry, University of Stuttgart	Germany
Piotr	Kowalski	Institute of Applied Radiation Chemistry	Poland
Justyna	Kozłowska	Theoretical Chemistry Group, Chemistry Department, Wroclaw University of Technology	Poland
Markus	Kraft	University of Cambridge	United Kingdom
Elfi	Kraka	Southern Methodist University	USA
Kasper	Kristensen	Department of Chemistry, Aarhus University	Denmark
Anna	Krylov	Dept. of Chemistry, USC	USA
Takako	Kudo	Gunma University	Japan
Noriyuki	Kurita	Toyohashi University of Technology	Japan
Jenő	Kürti	Institute of Physics, Eötvös University	Hungary
Werner	Kutzelnigg	Theoretical Chemistry, Ruhr Universitat Bochum	Germany
István	Ladjánszki	Department of Physical Chemistry and Material Science, Budapest University of Technology and Economics	Hungary
Antonio	Largo	Universidad de Valladolid	Spain
Ors	Legeza	Wigner Research Centre for Physics	Hungary
György	Lendvay	Institute of Materials andEnvironmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences	Hungary
Ingvar	Lindgren	Department of Physics, University of Gothenburg	Sweden
Shuhua	Li	Nanjing University	China
Wenjian	Liu	Peking University	China
Andre	Lomaka	Chair of Molecular Technology, Tallinn University of Technology	Estonia
Tian	Lu	University of Science and Technology Beijing	China
Gábor	Magyarfalvi	Institute of Chemistry, Eötvös Loránd University	Hungary
Haibo	Ma	Nanjing University	China

List of Participants cont'd

Given name	Family Name	Affiliation	Country
Jing	Ma	Nanjing University	China
Mariusz	Makowski	Faculty of Chemistry, University of Gdansk	Poland
Michal	Malček	Slovak University of Technology in Bratislava	Slovakia
Alejandro Fabián	Maldonado	IMIT - CONICET, UNNE	Argentina
Bhabani	Mallik	Department of Chemistry, Indian Institute of Technology Hyderabad	India
Glenn	Martyna	IBM TJ Watson Research Center	USA
Nicola	Marzari	EPFL	Switzerland
Marco	Masia	Boston University	USA
Aya	Matsuda	Ochanomizu University	Japan
Toru	Matsui	RIKEN Advanced Institute for Computational Science	Japan
Yu-ichiro	Matsushita	Max-Planck Institute of Microstructure Physics	Germany
Reinhard	Maurer	Technische Unversitaet Muenchen	Germany
Istvan	Mayer	Research Centre for Natural Sciences, Hungarian Academy of Sciences	Hungary
Sumit	Mazumdar	University of Arizona	United States
Arthitaya	Meeprasert	Chulalongkorn University	Thailand
Paul	Mezey	Memorial University of Newfoundland	Canada
Josef	Michl	Institute of Organic Chemistry and Biochemistry AS CR, v.v.i.	Czech Republic
Petr	Milko	Weizmann Institute of Science	Israel
Vladimir	Mironov	M.V.Lomonosov Moscow State University	Russia
Jan	Mitschker	University Oldenburg, Theoretical Chemistry	Germany
Noriyuki	Mizoguchi	Meiji Pharmaceutical University	Japan
Wataru	Mizukami	University of Bristol	UK
Nimrod	Moiseyev	Technion	Israel
Salvador	Moncho Escriva	Texas A&M University at Qatar	Qatar
Alena	Moon	Purdue University	USA
Hirotoshi	Mori	Ochanomizu University	Japan
Dmitry	Morozov	University of Jyvaskyla	Finland
Sebastian	Mosbach	Department of Chemical Engineering and Biotechnology, University of Cambridge	United Kingdom
Debashis	Mukherjee	Indian Association for the Cultivation of Science, Kolkata	India
Monika	Musial	University of Silesia	Poland

List of Participants cont'd

Given name	Family Name	Affiliation	Country
Bastien	Mussard	Universite de Lorraine	France
Ágnes	Nagy	University of Debrecen	Hungary
Péter	Nagy	Eötvös University	Hungary
Szilvia	Nagy	Széchenyi István University	Hungary
Katsumi	Nakagawa	MO BASICS Research	Japan
Hiromi	Nakai	Department of Chemistry and Biochemistry, Waseda University	Japan
Masayoshi	Nakano	Osaka University	Japan
Yutaka	Nakatsuka	RIKEN Advanced Institute for Computational Science	Japan
Gábor	Náray-Szabó	Laboratory of Structural Chemistry and Biology, Institute of Chemistry, Eotvos Lorand University	Hungary
Marco	Nascimento	Instituto de Química da UFRJ	Brazil
Fedor	Naumkin	UOIT	Canada
Ben	Nebgen	Purdue University	United States of America
Frank	Neese	Max-Planck-Institut fuer Chemische Energiekonversion	Germany
Michaela	Nekardova	Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic	Czech Republic
Karoly	Nemeth	Illinois Institute of Technology	USA
Alexander	Nemukhin	Lomonosov Moscow State University	Russian Federation
Sébastien	Nénon	University of Namur	Belgium
Cleanthes	Nicolaides	Theoretical and Physical Chemistry Institute	Greece
Yoshio	Nishimoto	Nagoya University	Japan
Anton	Nizovtsev	Nikolaev Institute of Inorganic Chemistry	Russia
Jozef	Noga	Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava	Slovakia
Kai	Nordlund	Department of Physics, University of Helsinki	Finland
Kaori	Noto	Kitasato University	Japan
Nadtanet	Nunthaboot	Mahasarakham University	Thailand
Gunnar	Nyman	University of Gothenburg	Sverige
Christian	Ochsenfeld	Theoretical Chemistry, University of Munich (LMU)	Germany
Roberto	Olivares-Amaya	Princeton University	United States
Carsten	Olm	Institute of Chemistry, Eötvös University (ELTE)	Hungary

List of Participants cont'd

Given name	Family Name	Affiliation	Country
Jeppe	Olsen	Aarhus University	Denmark
Hiroki	Otaki	RIKEN	Japan
Miho	Otsuka	Ochanomizu University	Japan
Takao	Otsuka	RIKEN Quantitative Biology Center	Japan
Nadia	Ouddai	univ-Hadj-lakhdar-Batna	algeria
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