



NEW CHALLENGES FOR AB INITIO THEORY IN MOLECULAR SCIENCE

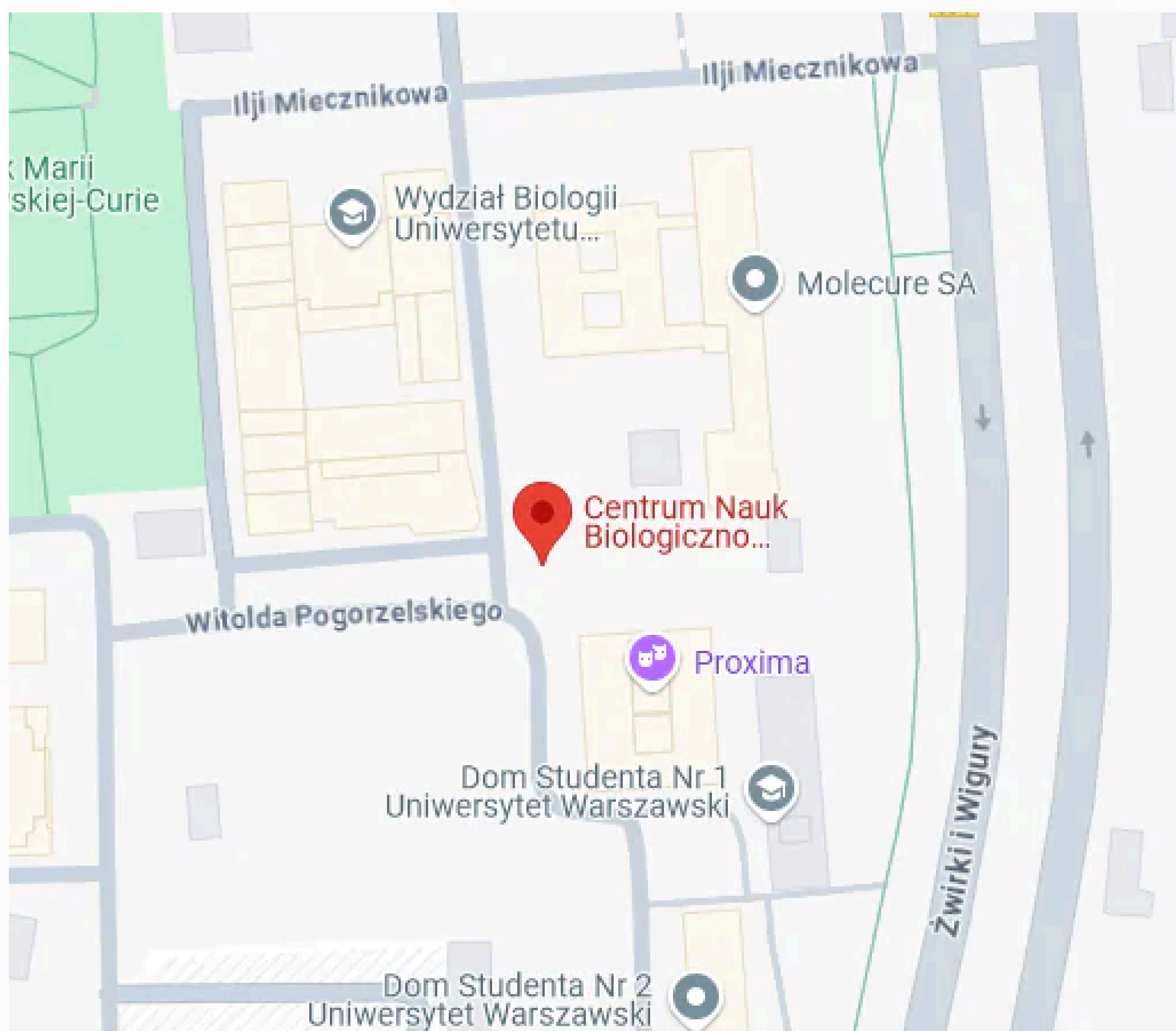
GENERAL INFORMATION

New Challenges for Ab Initio Theory in Molecular Science

1 -5 July 2025

The conference is an extended edition of the workshop “*Intermolecular Interactions: New Challenges for Ab Initio Theory*” (with the latest workshop taking place in 2023) and is dedicated to memory of **Bogumił Jeziorski**, who was an organizer of several recent editions of this workshop. The present conference, in addition to the subject of intermolecular interactions, includes topics such as accurate calculations for few-body systems, precision metrology of fluids, and theory of electron correlation.

Conference venue



The conference will be held at:

**Aula A+B,
Biological and Chemical
Research Centre**

University of Warsaw
Żwirki i Wigury 101
02-089 Warsaw, Poland



Organizing committee

Grzegorz Chałasiński, University of Warsaw, Poland

Berta Fernández Rodríguez, University of Santiago de Compostela, Spain

Michał Lesiuk, University of Warsaw, Poland

Krzysztof Szalewicz, University of Delaware, USA

GENERAL INFORMATION

New Challenges for Ab Initio Theory in Molecular Science

Bogumił Jeziorski — life and work

Bogumił Jeziorski was born on April 29, 1947, and passed away on September 15, 2023, at the age of 76. He spent his entire career at the Faculty of Chemistry, University of Warsaw, where he earned his MSc in 1969, PhD in 1975, and DSc in 1982. He was appointed full professor in 1991. Throughout his career, he held visiting positions at several institutions, including University of Delaware, Radboud University Nijmegen, University of Waterloo, University of Florida, and University of Utah.



Bogumił Jeziorski authored approximately 160 scientific publications spanning a broad spectrum of topics in physics and chemistry. His exceptional breadth of knowledge, coupled with a rare talent for generating original scientific ideas, led to fundamental contributions across several research domains. Among his most influential achievements was the development of symmetry-adapted perturbation theory (SAPT), including a practical framework applicable to arbitrary molecular systems, now widely used in quantum chemistry. Another major focus of Bogumił's research was coupled cluster (CC) theory. He introduced the state-universal (Hilbert-space) exponential ansatz for the wave operator, enabling accurate treatment of open-shell atoms and molecules. He also made key contributions to explicitly correlated CC methods based on Gaussian geminals. He was equally engaged in high-precision ab initio calculations for small atoms and molecules. His work included studies of exotic systems with muons, molecular effects in the beta decay of tritium, and interaction-induced properties of helium gas. Notably, the latter contributed to the 2019 redefinition of the International System of Units (SI). Bogumił received numerous honors for his scientific contributions, including the medal of the International Academy of Quantum Molecular Science (1987) and the Prize of the Foundation for Polish Science (2000), the most prestigious scientific award in Poland. He deeply valued collaboration - remarkably, only one of his publications is single-authored. He mentored a large group of PhD students, many of whom now hold faculty positions at leading academic institutions.

Bogumił will be remembered as an exceptional scientist - curious, active, and productive until the very end - and, just as importantly, as an extraordinary human being.

GENERAL INFORMATION

New Challenges for Ab Initio Theory in Molecular Science

Invited speakers

- **Ad van der Avoird**, Radboud University, Nijmegen, Netherlands
- **Zlatko Bačić**, New York University, New York, USA
- **Rodney Bartlett**, University of Florida, USA
- **Małgorzata Biczysko**, University of Wrocław, Poland
- **Tucker Carrington Jr.**, Queen's University, Kingston, Ontario, Canada
- **Attila G. Császár**, Eötvös Loránd University, Budapest, Hungary
- **Piotr Froelich**, Uppsala University, Sweden
- **Martin Head-Gordon**, University of California, Berkeley, USA
- **Teresa Head-Gordon**, University of California, Berkeley, USA
- **Gerrit C. Groenenboom**, Radboud University, Nijmegen, Netherlands
- **Trygve Helgaker**, University of Oslo, Norway
- **Piotr Jankowski**, Nicolaus Copernicus University, Toruń, Poland
- **Georg Jansen**, University of Duisburg-Essen, Germany
- **Kenneth Jordan**, University of Pittsburgh, USA
- **Tatiana Korona**, University of Warsaw, Poland
- **Nancy Makri**, University of Illinois at Urbana-Champaign, USA
- **Edit Mátyus**, Eötvös Loránd University, Budapest, Hungary
- **Alston J. Misquitta**, Queen Mary University of London, United Kingdom
- **Monika Musiał**, University of Silesia, Katowice, Poland
- **Hiroshi Nakatsuji**, Kyoto University, Japan
- **Jozef Noga**, Comenius University, Bratislava, Slovakia
- **Marcel Nooijen**, University of Waterloo, Canada
- **Konrad Patkowski**, Auburn University, USA
- **Krzysztof Pachucki**, University of Warsaw, Warsaw, Poland
- **Jiří Pittner**, Academy of Sciences of the Czech Republic, Prague, Czechia
- **Rafał Podeszwa**, University of Silesia, Katowice, Poland
- **Michał Przybytek**, University of Warsaw, Poland
- **Joachim Sauer**, Humboldt University, Berlin, Germany
- **Lyudmila Slipchenko**, Purdue University, West Lafayette, USA
- **Alexandre Tkatchenko**, University of Luxembourg, Luxembourg
- **Michał Tomza**, University of Warsaw, Warsaw, Poland
- **Piotr Wcisło**, Nicolaus Copernicus University, Toruń, Poland
- **Hans-Joachim Werner**, University of Stuttgart, Germany
- **Weitao Yang**, Duke University, Durham, USA
- **Dominika Zgid**, University of Michigan, USA
- **Piotr Żuchowski**, Nicolaus Copernicus University, Toruń, Poland

GENERAL INFORMATION

New Challenges for Ab Initio Theory in Molecular Science

Topics

- Fundamentals of intermolecular interactions
- New developments of density functional theory (DFT) and its applications in theory of intermolecular interactions
- Theory of electron correlation including coupled cluster methods and post-DFT approaches
- Methods applying explicitly-correlated basis sets
- Ultra-high accuracy methods for few-body systems
- Intermolecular interaction in ultra-cold physics and chemistry
- Nonreactive nuclear dynamics of van der Waals clusters
- Open-shell van der Waals clusters
- Applications to systems with dozens or hundreds of atoms
- Applications to soft condensed matter

Extra information for participants



The book of abstracts can be found under the following link:
ncaitms.chem.uw.edu.pl/wp-content/uploads/sites/236/2025/06/book-of-abstracts.pdf
Abstracts are ordered alphabetically.

Wi-fi: CNBC-PUB

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New Challenges for Ab Initio Theory in Molecular Science

Types and lengths of the presentations

- 1) Invited talk: 40 min (35 min talk + 5 min for discussion);
- 2) Contributed talk: 20 min (17-18 min talk + 2-3 min for discussion);
- 3) Poster presentation (two poster sessions: Wed, 2 July and Thu, 3 July);

Guidelines for oral presentations

- 1) Please upload a copy of your presentation to the local computer **at least one session in advance**. You can provide us your slides on a USB drive or (preferably) by sending them via mail to: p.michalak13@uw.edu.pl. Before your session you will be able to check if your slides display correctly. Unfortunately, due to a large number of talks you cannot use your own computer to project slides.
- 2) Speakers will use the on-ear microphone available in the conference room. Handheld microphones will be used by the chairs and technical support only.
- 3) The computer in the conference room has the following software installed: Microsoft Powerpoint, Adobe Reader DC, Apple Keynote. However, we strongly encourage all speakers to prepare their final slides in PDF format.
- 4) The recommended aspect ratio for the slides is 16:9. Please let us know in advance if your slides have a different aspect ratio.

Guidelines for poster presentations

- 1) The poster stands available at the conference are able to support posters of size A0. Any smaller size will obviously work as well.
- 2) If your poster presentation is in the first session (Wed, 2 July) you can put up your poster at the very beginning of the conference. However, you have to take it down by morning Thu, 3 July at the latest. If your presentation is in the second session (Thu, 3 July) you can put up your poster in the afternoon and it can stay there until the end of the conference.
- 3) The organizers will provide equipment needed to put posters on the stands.

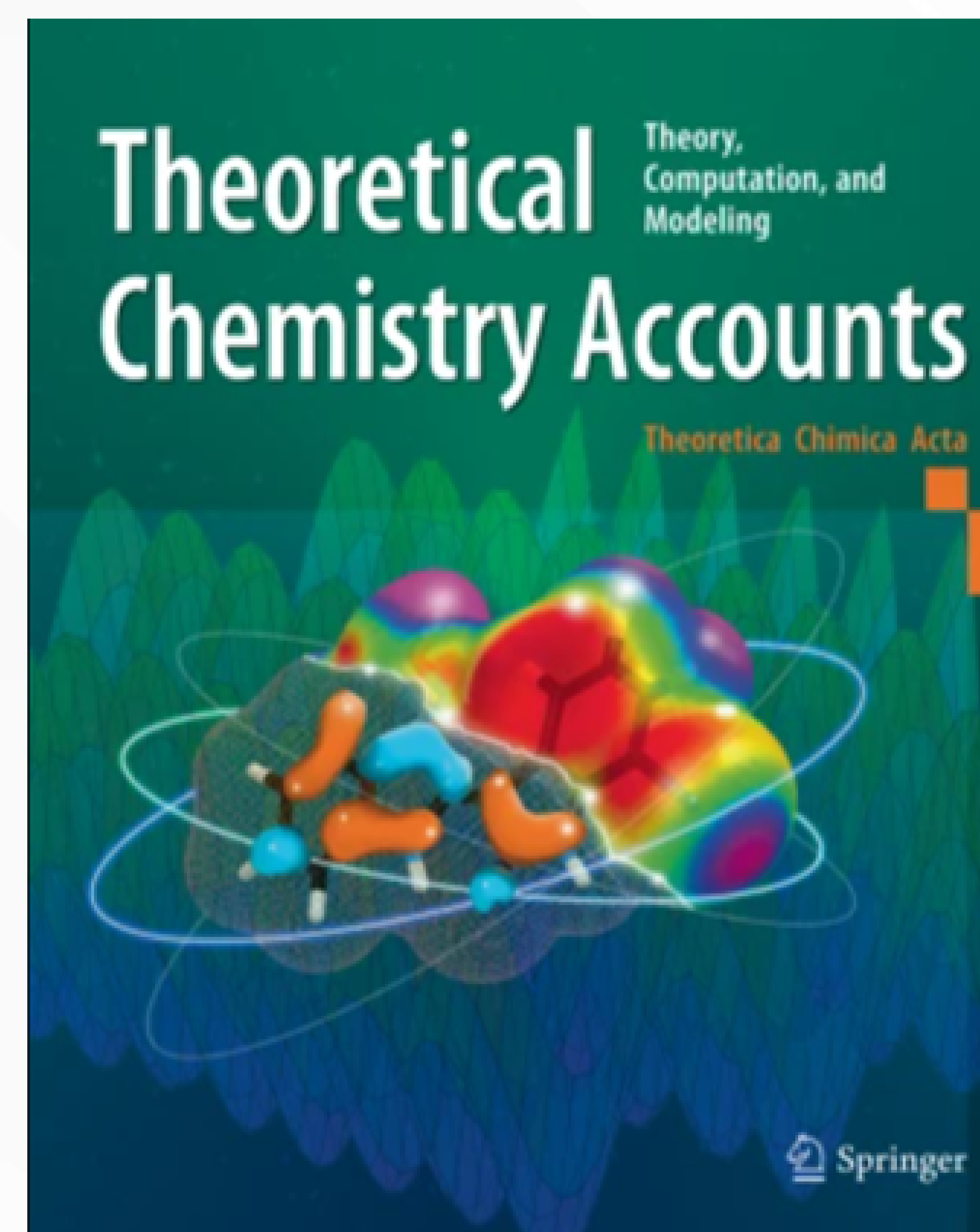
GENERAL INFORMATION

New Challenges for Ab Initio Theory in Molecular Science

Special Issue Announcement

We are pleased to announce a special issue of *Theoretical Chemistry Accounts* organized in memory of **Bogumił Jeziorski**. All participants of the conference, including those with oral or poster presentations, are invited to submit research papers to this special issue. The conference organizers will serve as Guest Editors and will be joined by Associate Editor Piotr Piecuch, who will represent the journal as Lead Editor for this issue.

Submissions covering all topics within the scope of *Theoretical Chemistry Accounts* are welcome; however, the editors are particularly interested in contributions related to the research interests of **Bogumił Jeziorski**, including:



- fundamentals of intermolecular interactions;
- new developments in density functional theory (DFT) and its applications to intermolecular interactions;
- theory of electron correlation, including coupled-cluster methods and post-DFT approaches;
- methods employing explicitly correlated basis sets;
- ultra-high accuracy approaches for few-body systems;
- intermolecular interactions in ultracold physics and chemistry;
- nonreactive nuclear dynamics of van der Waals clusters;
- open-shell van der Waals clusters;
- applications of molecular electronic structure methods to systems containing dozens or hundreds of atoms, as well as to soft condensed matter.

As with all submissions to *Theoretical Chemistry Accounts*, manuscripts submitted to this special issue will undergo a peer-review process to ensure the highest quality of accepted papers.

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Tuesday 01.07.2025

08:45 - 09:00

Opening

Session I: Coupled cluster theory

**Chairperson
I. Grabowski**

09:00 - 09:40

Rodney J. Bartlett

Correlated Orbital Theory: An Alternative
and Complement to Kohn-Sham DFT

09:40 - 10:20

Monika Musiał

The Coupled Cluster Method Applied to the Study of Open-Shell
Systems Based on the Closed-shell Reference Function

10:20 - 11:00

Marcel Nooijen

Configurational Coupled Cluster

Coffee Break

11:30 - 12:10

Trygve Helgaker

Variational reformulation of molecular properties
in electronic-structure theory

12:10 - 12:50

Jiří Pittner

Coupled Cluster Methods Externally Corrected by DMRG

12:50 - 13:30

Jozef Noga

Hartree-Fock via Variational Coupled Cluster Singles
with Natural Virtual Orbitals

Lunch Break

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Tuesday 01.07.2025

Session II: Intermolecular interactions, part 1

Chairperson
B. Lesyng

14:30 - 15:10

Kenneth D. Jordan

Importance of Charge-Flow Polarization in Polyaromatic Hydrocarbons:
Extrapolation to the Image Potential of Graphene

15:10 - 15:50

Konrad Patkowski

Decomposing Noncovalent Intramolecular Interactions

15:50 - 16:30

Georg Jansen

Revamping the Formalism of Intermolecular
Perturbation Theory

Coffee Break

17:00 - 17:40

Piotr S. Żuchowski

Response Theory and Molecular Interactions

17:40 - 18:20

Alston J. Misquitta

Symmetry-adapted Relaxation Theory (SART): a SAPT-Inspired Theory
with Infinite-order Induction Relaxation of Monomers

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Wednesday 02.07.2025

Session III: Intermolecular interactions, part 2

Chairperson
B.Fernández

09:00 - 09:40

Lyudmila V. Slipchenko

Modeling Noncovalent Interactions with
the Effective Fragment Potential Method

09:40 - 10:20

Teresa Head-Gordon

Advances in Force Fields for Molecular Simulation
and Foundation Models

10:20 - 11:00

Tatiana Korona

Symmetry-adapted Perturbation Theory with Monomers Described
on the Coupled Cluster Theory level – theory, challenges, and applications

Coffee Break

Session IV: DFT and beyond

Chairperson
M. Hapka

11:30 - 12:10

Weitao Yang

DFT: Advances in Functional Approximations
and in Theory for Excited States

12:10 - 12:50

Dominika Zgid

Homotopy Continuation Method for
Solving Dyson Equation Fully Self-Consistently

12:50 - 13:30

Krzysztof Szalewicz

Remembering Bogumił Jeziorski and his breakthrough
insights in theory of electron correlation and of intermolecular forces

Lunch Break

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Wednesday 02.07.2025

Contributed talks I

Chairperson
G. Chałasiński

14:30 - 14:45

Marlene Bosquez Fuentes

Rovibrational Quantum Dynamics of Simple
Van der Waals Complexes

14:45 - 15:00

Nikhila Ambika Chandran

Complete Insensitivity to *Ab Initio* Data: A New Perspective on Modeling
Collision-Induced Absorption of Noble Gas Atoms

15:00 - 15:15

Humahuti Dihingia

Towards Accurate Description of Intermolecular Induction

15:15 - 15:30

Anderson Exlonk Gil Peláez

Quantum-Informed Machine Learning for Predicting
Fluorescence Quantum Yield

15:30 - 15:45

Katarzyna M. Krupka

Single- and Multi-Reference Approaches for Open-Shell
Metal Cluster-PAH Interactions. UMP2C and RS2CC Methods

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Wednesday 02.07.2025

Poster session I				16:00–18:00	
P1	Iulia Emilia Brumboiu Computational RIXS: Benchmark and Applications to Organic Molecules Used in Photovoltaics	P9	Marta Gałyńska A Domain-Based Charge-Transfer Analysis of the First Excited State Calculated with EOM-PCCD+S		
P2	Koushik Chatterjee Long-range Dispersion Interaction Between Atoms and Molecules in Electronically Excited States	P10	Piotr Gniewek Interactions of Atomic Ions with Diatomic Molecules		
P3	Dominik Cieśliński First-Order Symmetry-Adapted Perturbation Theory with Double Exchange for Multireference Systems	P11	Marcin Gronowski The Electronic Structure of ALF Molecule		
P4	József Csóka Advancing Quantum Embedding Methods for Modeling Catalytic Environments: Local Approximations and Forces	P12	Tarun Gupta Induction Energy for Molecules in Excited State - a Comparison of Induction Energy from Finite-Field and SAPT		
P5	Janusz Cukras Theoretical Prediction of Magneto-Chiral Dichroism for Helicenes and Other Chiral Organic Molecules	P13	Mikolaj Gurba Effects of Base Stacking on Excited States in Nucleobase		
P6	Dawid Dąbrowski The Excited Electronic States of the Helium Dimer Including Adiabatic and Relativistic Effects	P14	Michał Hapka Correcting Basis Set Incompleteness in Wave Function Correlation Energy by Dressing Electronic Hamiltonian with an Effective Short-Range Interaction		
P7	Achintya Kumar Dutta A New Perturbative Triples Correction Scheme to Unitary Coupled Cluster Method	P15	Gaurav Harsha Describing Disorder and Correlation – Coherent Potential Approximation with Bloch Gaussians		
P8	Reinhold Fink Molecular Orbital Pair Contributions to the Exchange Repulsion Energy Explain the Conundrum of π -Interactions	P16	Hamza Hendaoui Insights into Rotational (De-)excitation of Interstellar Calcium Dicarbide (c-CaC ₂) induced by Helium Collisions		

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Wednesday 02.07.2025

Poster session I				16:00–18:00	
P17	James Hooper “A Decomposition of Interaction Energies in Periodic Models and its Insights into Bonding and Descriptors ”	P23	Tymon Kilich Ultracold Highly Polar KAG and CSAG Molecules: Electronic Structure and Optical Formation		
P18	Munavvar Husain “Exploring Excited Molecular States via Localized Orbital Locator: A Quantum Topology Analysis of Charge Transfer in the Ethylene–Tetrafluoroethylene Complex”	P24	Adrianna Kruk Predicting Molecular Excitations induced by a High-Velocity Massive Charged Particle		
P19	Benjamin Adebajo Ikuesan “Selected Excited-State Rovibrational and Electronic Structures of the Carbon Monoxide Molecule (Preliminary Result)”	P25	Deepak Kumar Self-Consistent-Field Solution for Unstable Anions		
P20	Joanna Jankowska “Molecular-Dynamics Assisted Modeling of Fluorescence Decay in MR-TADF Emitters”	P26	Marta Łabuda Theoretical Investigations on Fragmentation of Dihydropyran Molecule(C5H8O)		
P21	Dorota Rutkowska-Żbik DFT Studies on Cu Single Atom and Sub-Nanometer Copper Clusters Deposited on TiO ₂ for H ₂ Generation	P27	Hela Ladjimi Radioactive RaAg ⁺ Molecular Ion: Electronic Structure, Formation Schemes, and Prospects for Precision Measurements		
P22	Almaz Khabibrakhmanov Noncovalent Interactions in Density Functional Theory: All the Charge Density we do not see	P28	Jakub Lang Third Virial Coefficients of Helium Gas		

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Thursday 03.07.2025

Session VI: Explicitly-correlated methods

Chairperson
M. Lesiuk

09:00 - 09:40

Hans-Joachim Werner

Accurate Calculations of Non-Covalent Interactions
Using PNO-LCCSD(T)-F12

09:40 - 10:20

Michał Przybytek

Weak Orthogonality Formulation of the Coupled Cluster
Theory with Explicitly Correlated Slater Functions

10:20 - 11:00

Edit Mátyus

The ABC of Triplet Helium Dimer

Coffee Break

Session VII: Soft condensed phase

Chairperson
W. Skomorowski

11:30 - 12:10

Nancy Makri

Small Matrix and Modular Path Integral Methods
for Quantum Dynamics

12:10 - 12:50

Joachim Sauer

Ab Initio Free Energy Simulations with Chemical Accuracy
– Water in Nanoporous Materials

12:50 - 13:30

Małgorzata Biczysko

Validation of Clustering for Quantum-Based Refinement
of Biomacromolecules

Lunch Break

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Thursday 03.07.2025

Contributed talks II

Chairperson
R. Fink

14:30 - 14:45

Rony Letona

Automatic Temperature-Dependent Lattice Free
Energies of Disordered Molecular Crystals

14:45 - 15:00

Omar Rodríguez

Cutting-Edge Machine Learning Approaches for Efficient
and Accurate Reaction Network Analysis

15:00 - 15:15

Edoardo Vanich

Symmetry-Adapted Relaxation Theory (SART):
First-Quantization Hartree-Fock Theory and Implementation

15:15 - 15:30

Bruno von Bruening

New Approach for Distributed Multipole Assessment:
Why You Should use LISA?

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Thursday 03.07.2025

Poster session II				15:50-17:50	
P29	Judith Leson Long-Range Intermolecular Interactions Involving Excited States of Benzene	P37	Kamil Nalikowski Embedded Cluster Approach to Describe the Electronic Structure of Doped Crystals		
P30	Bogdan Lesyng Is the Development of Quantum Modeling Methods Subject to the Laws of Evolution?	P38	Fedor Naumkin Non- and Reactive Structural Evolution of Intermolecular Systems		
P31	Dibyendu Mahato Green’s Function Integrals with Spherical Gaussian and Plane-Wave-Modulated Basis Functions	P39	Grzegorz Niedzielski Computational Studies of Molecular Crystal Excited States Using Periodic DFT+U Calculations		
P32	Bartosz Majewski Theoretical Investigations on Fragmentation of Dihydropyran Molecule(C5H8O)	P40	Jan Okoński Accurate Ab initio Calculations of Interaction Potentials of the Alkali and Alkaline-Earth Metal Hydrides		
P33	Bilel Mehnen Rotational Excitation and De-Excitation of the Interstellar Propargyl (H ₂ CCCH ⁺) Cation by Collisions with Helium Atoms	P41	Khanh Ngoc Pham Accuracy of Approximate Methods for Describing Many-Body Contributions of Binding Energies of Molecular Crystals		
P34	Piotr Michalak Rank-Reduced Equation-of-Motion Coupled Cluster Methods with Triple Excitations	P42	Florian Pimpel Rank-reduced coupled cluster theory for energy gradients		
P35	Masato Morita Ab initio Calculations of Feshbach Resonances in Ultracold Collisions Between Rb and AlF	P43	Saikat Roy Resonance Widths of Autoionizing Rydberg States via Projections Technique Combined with EOM-CCSD Method		
P36	Tymoteusz Mrozek Accurate Dynamic Polarizabilities in Excited States by Means of ECG Basis Functions	P44	Igor Sawicki Improving Double Hybrid Functionals via Regularized Second-Order Perturbation Theory		

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Thursday 03.07.2025

Poster session II				15:50-17:50	
P45	Jonathan Scherlitzki Ultrafast Electronic Chirality Flips in the Triatomic Molecule NSF: a New Application of <i>Ab Initio</i> Quantum Chemistry	P52	Bartosz Tyrcha Recent Developments in Second-Quantization-Based Symmetry-Adapted Perturbation Theory		
P46	Leonid Shirkov Application of SAPT for Constructing Transferable Intermolecular Potentials	P53	Munkhorgil Wang Comparing Fully Self-Consistency GW (scGW) and Fully Self-Consistency Vertex-Corrected GW (scGWF) with Tensor Hypercontraction		
P47	Aditi Singh Universally Applicable Range-Separation Tuning	P54	Dahvyd Wing Approximating Pauli Exchange-Repulsion: a Transferable Model Based on Electron Density		
P58	Monika Srebro-Hooper Exploring Non-Covalent Interactions in Supramolecular Systems Using Density Functional Theory	P55	Henryk Witek Progress In Exact Analytical Solution of Schrödinger Equation of the Helium Atom		
P49	Korutla Srikanth Complex Potential Energy Surfaces for Penning Ionization Through Complex Basis Functions	P56	Mateusz Witkowski Ultrafast Correlation-Energy Estimator		
P50	Krystyna Syty Multi-level Coupled Cluster Description of Crystal Lattice Energies	P57	Emil Żak Sharpening Tools for Drug Discovery: Size-Consistent Brillouin–Wigner Second-Order Perturbation Theory Calculations for Molecular Docking and Quantum Algorithms for Modeling Accurate Electronic-Vibrational-Rotational Dynamics		
P51	Aleksandra Tucholska Enhanced DMRG-AC Approach for Efficient Treatment of Strongly Correlated Systems				

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Friday 04.07.2025

Session IX: Dispersion in density functional theory

Chairperson
M. Pecul-Kudelska

09:00 - 09:40

Martin Head-Gordon

Some Recent Advances in Density Functional Theory:
Three Short Stories

09:40 - 10:20

Alexandre Tkatchenko

Quantum Drude Oscillators for Accurate Modeling of non-Covalent
Interactions in Molecules and Condensed Matter

10:20 - 11:00

Rafał Podeszwa

Dispersionless density functional with physically
correct dispersion correction

Coffee Break

Session X: Ultra-high accuracy calculations

Chairperson
A. Kaczmarek-Kędziera

11:30 - 12:10

Hiroshi Nakatsuji

Exact Scaled Schrödinger Equation Theory Combined with
SAC/SAC-CI Theory and Electrostatic Force Theory

12:10 - 12:50

Krzysztof Pachucki

QED Theory of $X^1\Sigma_g^+$ Energy Levels of H_2

12:50 - 13:30

Piotr Froelich

Rearrangement Collisions of anti-Hydrogen Atoms and Ions with Positronium,
of Interest for Experiments on Fundamental Physics at CERN

Lunch Break

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Saturday 05.07.2025

Session XI: Quantum nuclear dynamics, part 1

Chairperson
B. Braams

09:00 - 09:40

Tucker Carrington Jr.

Exceptionally Accurate ro-Vibrational Energy Levels
and Tunnelling Splittings of Water Dimer

09:40 - 10:20

Ad van der Avoird

Para-Ortho H₂ Conversion by Collisions with O₂ and NO

10:20 - 11:00

Piotr Jankowski

How Important are Monomer-Flexibility Effects
for Spectra of Van der Waals Clusters?

Coffee Break

11:30 - 12:10

Piotr Wcisło

Towards trapping cold hydrogen molecules

12:10 - 12:50

Michał Tomza

Quantum Control of Ultracold Atom-Ion
and Atom-Molecule Collisions

Lunch Break

PROGRAM

New Challenges for Ab Initio Theory in Molecular Science

Saturday 05.07.2025

Session XII: Quantum nuclear dynamics, part 2

Chairperson
M. Biczysko

14:30 - 15:10

Zlatko Bačić

Water Trimer: Rigorous Twelve-Dimensional Quantum Calculations of Intermolecular Vibration-Tunneling States and Low-Frequency Absorption Spectrum

15:10 - 15:50

Attila G. Császár

Quasistructural Molecules

15:50 - 16:30

Gerrit Groenenboom

Rotation-Vibration Inelastic Collision Rates

Closing

08:45	Opening												
09:00	I	Rodney Bartlett	III	Lyudmila Slipchenko	VI	Hans-Joachim Werner	IX	Martin Head-Gordon	XI	Tucker Carrington Jr.			
09:40		Monika Musiał		Teresa Head-Gordon		Michał Przybytek		Alexandre Tkatchenko		Ad van der Avoird			
10:20		Marcel Nooijen		Tatiana Korona		Edit Mátyus		Rafał Podeszwa		Piotr Jankowski			
11:00	Coffee Break												
11:30	II	Trygve Helgaker	IV	Weitao Yang	VII	Nancy Makri	X	Hiroshi Nakatsuji	XII	Piotr Wciśło			
12:10		Jiří Pittner		Dominika Zgid		Joachim Sauer		Krzysztof Pachucki		Michał Tomza			
12:50		Jozef Noga		* Krzysztof Szalewicz		Małgorzata Biczysko		Piotr Froelich		Lunch break			
13:30	Lunch break												
14:30	II	Kenneth Jordan	V	Graduate students talks	VIII	Graduate students talks	XII	Zlatko Bačić	XII	Attila G. Császár			
15:10		Konrad Patkowski											
15:50		Georg Jansen											
16:30	Coffee Break												
	Closing												

Topics of thematic sessions and lectures:

I	Coupled cluster theory
II	Intermolecular interactions (part 1)
III	Intermolecular interactions (part 2)
IV	DFT and beyond
*	Bogumił Jeziorski - life and work
VI	Explicitly-correlated methods
VII	Soft condensed phase
IX	Dispersion in density functional theory
X	Ultra-high accuracy calculations
XI	Quantum nuclear dynamics (part 1)
XII	Quantum nuclear dynamics (part 2)

