EuChemS CompChem 2023

European Conference on Computational & Theoretical Chemistry

"Exploring Molecular Space"

Presented by the
Division of Computational and Theoretical Chemistry

Olympic Museum
Thessaloniki, Greece
August 27-31, 2023

www.euchems-compchem.eu

Ένωση Ελλήνων Χημικών
Association of Greek Chemists

EuChemS
European Chemical Society

PROGRAM

Welcome

Dear colleagues,

On behalf of the European Chemical Society, I wish you a warm welcome to CompChem2023.

The European Chemical Society – in short EuChemS – is an overarching society at the European level with 50 national chemical societies and other organisations as members. Our mission is to nurture a platform for scientific discussion and provide an unbiased European voice on key policy issues in chemistry and related fields. In this way, EuChemS represents approximately 130,000 chemists from all over Europe.

Did you ever realize that by being a member of your national chemical society, you are a member of EuChemS too? If you are interested to learn more about EuChemS, feel free to sign up for our monthly newsletter EuChemS Magazine (www.magazine.euchems.eu), where we share information that is relevant for you.

The themes of this conference, ranging from Artificial Intelligence in Chemical Research to Computational Chemistry in Industry, are crucial in contemporary chemistry. In this field, it is especially important to remain on the cutting edge of innovative research – and occasions like this ensure the exchange of pioneering ideas. Therefore, I wish to express my gratitude to the EuChemS Division of Computational and Theoretical Chemistry for setting up such a wonderful conference.

While I have to remain in the Netherlands, I sincerely hope that you will participate in numerous exciting conversations, facilitate knowledge exchange, and make new connections with your colleagues in the field of computational chemistry and beyond in beautiful Thessaloniki.

I wish you a very enjoyable conference!

Floris Rutjes

Floris Rutjes
President of the European Chemical Society (EuChemS)

Dear colleagues,

On behalf of the Association of Greek Chemists, I welcome you to Thessaloniki and to the CompChem2023. The Association of Greek Chemists (AGC) is a scientific organization representing all Chemists in Greece and is member of the European Chemical Society and member of the chemical societies comprising Chemistry Europe.

AGC was founded in 1924 and since then has grown substantially, comprising at the moment of AGC has built a tradition in organizing international conferences, among which are the divisional conferences of EuChemS. In 2019, AGC has organized the 17th International Conference on chemistry and the Environment, which is the conference of the division of Chemistry and the Environment, in 2021 the conference on Green and Sustainable Chemistry, namely the conference of the Division of Green and Sustainable Chemistry, and this year the 14th European Conference on computational and theoretical chemistry.

We are therefore grateful to our members and delegates to the EuChemS divisions for taking such initiatives and organizing such high-profile events in our country.

This conference will serve as a platform for scientists to highlight their recent research findings in theoretical and computational chemistry, which certainly find applications to all other aspects of chemistry and other sciences as well. From this perspective, it will be a very stimulating conference for all chemists and I hope that several scientists from all over the world will attend. I wish to every participant an exciting and intriguing conference, full of interesting talks and fruitful discussions and I hope that you will find some time to discover the beauties and the history of Thessaloniki and Northern Greece.

Sincerely,

Ioannis Katsoyiannis
President of the Association of Greek Chemists

Welcome

Dear Colleagues and Friends,

It is a pleasure to welcome you to the EuChemS CompChem 2023, the flagship event of the European Chemical Society Division of Computational and Theoretical Chemistry (DCTC) from Sunday 27th August to Thursday 31st August, 2023, which takes place the Olympic Museum of Thessaloniki, Greece under the auspices of the Association of Greek Chemists.

EuChemS CompChem 2023 addresses key areas in computational and theoretical chemistry:
- Electronic Structure: Theory and Applications
- Artificial Intelligence in Chemical Research
- Materials Design
- Biomolecular Systems
- Computational Chemistry in Industry

Computational and theoretical chemistry have revolutionized the study of molecular events, the design and characterization of new materials, and the discovery of new drugs. The steady and consistent development of new theoretical methods and algorithms, access to massive compute resources, and breakthroughs in the processing of data using AI approaches allows the prediction of molecular properties at a level of accuracy required in industrial research, bringing computational chemistry to a new era.

We are particularly thrilled that the conference received an overwhelming response with over 300 participants from 33 countries, presenting 5 Keynote Lectures, 16 Invited Lectures, 40 Invited Contributions, 22 Short Communications, and 182 Poster Presentations contributing to a rich scientific program. The first day of the conference also features Opening Lectures by Prof. Michele Parrinello, Gold Medalist EuChemS 2020; Prof. Silvia Osuna, EuChemS Lecturer 2022, and our very own Chair of EuChemS-DCTC 2017-2022, Prof. Péter G. Szalay.

EuChemS CompChem 2023 presents the inaugural EuChemS Walter Thiel Award, an award recognizing biennially the outstanding scientific contributions of a young researcher based in a country affiliated to the EuChemS. The award is co-sponsored by Chemistry Europe, the German Chemical Society, the Swiss Chemcial Society, and the Max Planck Institut für Kohlenforschung. The inaugural award is presented to Dr. Felix Plasser of Loughborough University, UK. The Organizing Committee of EuChemS CompChem 2023 will also present a Lifetime Achievement Award to Prof. Hans Lischka. Moreover, three awards for outstanding poster presentations in each of the thematic sessions, as well as best contributed talk awards for outstanding contributed presentations will be given. Six fellowships to attend the EuChemS CompChem 2023 were granted as free registration fees to support students or early career scientists, kindly sponsored by CCP-BioSim.

Finally, I would like to extend our special thanks to the members of the organizing committee, who have worked tirelessly for the past year so that we can all be here today; to our scientific committee for ensuring the highest scientific standards; to our local organizing committee for tending to all meeting details; to EuChemS and the Association of Greek Chemists for providing the platform to organize this conference; to our DCTC delegates for engaging their local communities; to our sponsors for the financial assistance; to our media sponsors for disseminating the event; and last but not least to all of you for making this conference a success!

We are looking forward to an exciting EuChemS CompChem and wish you an enjoyable time at the historical and beautiful city of Thessaloniki.

Dr. Zoe Cournia
Chair, 2023 European Conference on Computational and Theoretical Chemistry
Treasurer, EuChemS DCTC
Senior Investigator, Biomedical Research Foundation Academy of Athens

Organizing Committee

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Assoc. Professor, Laboratory of Chemical and Environmental Technology,
Department of Chemistry, Aristotle University of Thessaloniki, Greece

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Sorbonne University, Paris, France

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Professor, University of Milano - Bicocca,
Italy

14:00-16:00	**Registrations**	
16:00	**Opening Remarks** • **Zoe Cournia,** Chair EuChemS Comp Chem 2023; Treasurer of EuChemS DCTC; Senior Researcher Biomedical Research Foundation Academy of Athens, Greece • **Ioannis Katsoyannis,** President of the Association of Greek Chemists; Assoc. Professor, Laboratory of Chemical and Environmental Technology, Department of Chemistry, Aristotle University of Thessaloniki, Greece • **Hans Peter Lüthi,** co-Chair EuChemS Comp Chem 2023; Treasurer of EuChemS; Executive Board Member Swiss Chemical Society • **Tanja van Mourik,** President of EuChemS DCTC; Reader, School of Chemistry, University of St Andrews, UK • **Michail Sigalas,** Professor and Director, Laboratory of Quantum and Computational Chemistry, Department of Chemistry, Aristotle University of Thessaloniki	
16:30-18:15	**Opening Session** Chair: **Zoe Cournia**	
	16:30	**Opening Lecture: Michele Parrinello,** Italian Institute of Technology, Italy Gold Medalist EuChemS 2020 The physics of catalysis
	17:15	**Chemistry Europe Lectureship: Silvia Osuna,** University of Girona, Spain EuChemS Lectureship 2022 Computational enzyme design: Towards the development of fast yet accurate approaches
	17:45	**IL: Péter G. Szalay,** ELTE Eötvös Loránd University, Institute of Chemistry Immediate Past President EuChemS DCTC Ab initio fragment models for accurate excimer potential energy surfaces
18:15	**Coffee | Tea Break**	
18:35-19:30	**EuChemS Walter Thiel Award Ceremony & Award Lecture** Chair: **Hans Peter Lüthi**	
	18:35-18:45	**Walter Thiel Award Ceremony** **Hans Peter Lüthi,** EuChemS Treasurer, Swiss Chemical Society **Tanja van Mourik,** President EuChemS DCTC **Sarah-Lena Gombert,** MPI KoFo **Péter G. Szalay,** Immediate Past President EuChemS DCTC
	18:45-19:30	**Walter Thiel Award Lecture: Felix Plasser,** Loughborough University, UK New Analysis Tools for Excited-State Quantum Chemistry: From Numbers to Chemical Insight
19:30	**Welcome Apéro**	

08:45-10:30	**Electronic Structure: Theory and Applications** Chair: **Péter G. Szalay**	
	08:45	**KL: Katarzyna Pernal,** Lodz University of Technology, Poland Beyond-active-space electron correlation for molecules in excited states
	09:30	**IL: Sandra Luber,** University of Zürich, Switzerland Pushing the boundaries for computational spectroscopy and excited states in the condensed phase
	10:00	**IL: Marie-Liesse Doublet,** ICGM - CNRS, France Materials for Energy Storage: Challenges and Related Issues
10:30	**Coffee | Tea Break**	
11:00-13:10	**Electronic Structure: Theory and Applications** Chair: **Péter G. Szalay**	
	11:00	**IL: Sotiris Xantheas,** Pacific Northwest National Lab, USA The Many-Body Expansion in Chemistry
	11:30	**IL: Demeter Tzeli,** National and Kapodistrian University of Athens, Greece Electronic Structure and Chemical Bonding in systems containing of transition metals
	12:00	**IC: Jan Martin,** Weizmann Institute of Science, Israel Basis set convergence of post-CCSD(T) corrections to high-accuracy thermochemistry reconsidered: the power of lambda
	12:20	**IC: Herbert Fruchtl,** University of St Andrews, UK Flick the switch – a candidate molecule for molecular electronics
	12:40	**IL: Hans Lischka,** Texas Tech University, USA **DCTC Lifetime Achievement Award** Solvent-enhanced symmetry-breaking induced by low-frequency vibrations in the covalently bound tetracene dimer leading to singlet-fission
13:10-14:30	**Lunch**	
14:30-16:25	**Materials Design** Chair: **Mercè Deumal**	
	14:30	**KL: Jacqueline Cole,** Department of Physics, University of Cambridge, UK Data-Driven Materials Discovery
	15:15	**IL: Benoît Champagne,** University of Namur, Belgium Predicting the Second-Order Nonlinear Optical Responses of Organic Materials in Complex Environments: The Role of Dynamics
	15:45	**IC: Cristina Trujillo,** University of Manchester, UK In Silico Design in Organocatalysis
	16:05	**IC: Carles Bo,** ICIQ, Spain New graph-based tools for taming complex reaction networks
16:25-17:00	**Coffee | Tea Break**	

Invited Contribution: **IC** | Invited Lecture: **IL** | Keynote Lecture: **KL** | Short Communication: **SC**

17:00-17:50	**Materials Design** Chair: **Radu Silaghi-Dumitrescu**	
	17:00	**IL: Maria João Ramos,** University of Porto, Portugal Biodegrading Plastic
	17:30	**IC: Anton Stasyuk,** University of Girona, Spain Aromaticity controls the photoinduced electron transfer in host-guest complexes of nanohoops
18:00-18:50	**Short Communications** Chairs: **Peter Reinhardt, Radu Silaghi-Dumitrescu**	
	Electronic Structure: Theory and Applications	
	18:00	**SC: Eline Desmedt,** Vrije Universiteit Brussel, Belgium Designing Nonlinear Optical Redox Switches with Inverse Molecular Design: the Synergy between Core-modifications and Meso-substitutions
	18:05	**SC: Marco Mendolicchio,** Scuola Normale Superiore, Italy New Challenges in Computational Spectroscopy
	18:10	**SC: Josianne Owona,** Donostia International Physics Center, Spain Theoretical modelling of mechanoluminescent properties of pyridylvinylanthracene crystals
	18:15	**SC: Nora Gildemeister,** University of Cologne, Germany Modelling charge transport properties of dipolar self-assembly merocyanines: the role of static and dynamic disorder
	18:20	**SC: Jordan Rio,** Université Claude Bernard Lyon 1, France Unveiling the Dynamic Structure of Organozincs in THF: Elucidating solvent effects with Molecular Dynamics and X-Ray Absorption Spectroscopies
	Materials Design	
	18:25	**SC: Pierre Beaujean,** University of Namur, Belgium Ruthenium Complexes as a Test System to Unravel the Symmetry Effects on the Second-Order Nonlinear Optical Responses of Molecular Switches
	18:30	**SC: Manuel Pérez Escribano,** Universidad de Valencia, Spain Computational study into the formation of tin halide perovskite nanostructures
	18:35	**SC: Anthony Payne,** University of Surrey, UK Growth and reactivity of Hexagonal Boron Nitride
	18:40	**SC: Jakob Brauer,** University of Bremen, Germany Deducing desirable properties of porous materials for the adsorption of complex organic molecules by employing an efficient hierarchical screening approach
	18:45	**SC: Lyuben Borislavov,** Bulgarian Academy of Sciences, Institute of General and Inorganic Chemistry, Bulgaria Cheminformatics-Aided Prediction of Degradation Reaction Products in Energy Storage Materials
18:50-20:30	**Poster Session I**	

08:45-11:00	**Computational Chemistry in Industry** Chair: **Michael Edmund Beck**	
	08:45	**KL: Tobias Morawietz / Sadra Kashe Ol Gheta,** Bayer AG, Pharmaceuticals R&D, Computational Molecular Design, Germany AIQU: Bridging Artificial Intelligence and Quantum Chemistry for Improved Molecular Property Prediction in Industrial R&D
	09:30	**IL: Christoph Riplinger,** FAccTs GmbH, Germany Deciphering key interactions of ligand binding to biomolecular targets using high-level quantum mechanical methods
	10:00	**IC: Miles Pemberton,** AstraZeneca, UK Predicting the Future of our Medicines: Applying AI/ML to Investigate the Link Between Molecular Structures and their Transcriptomic Signatures
	10:20	**IC: Albert Sabadell-Rendón,** ICIQ – Institute of Chemical Research of Catalonia, Spain AMUSE - Automated MUltiscale Simulation Environment
	10:40	**IC: George Fanourgakis,** Aristotle University of Thessaloniki, Greece Machine Learning as a tool for predicting gas adsorption by Metal Organic Frameworks
11:00-11:20	**Coffee | Tea Break**	
11:20-13:00	**Computational Chemistry in Industry** Chair: **Michael Edmund Beck**	
	11:20	**IL: Maria Jose Aliaga Gosalvez,** Software for Chemistry & Materials BV (SCM), Netherlands Collaborating with SCM: (Horizon Europe) opportunities
	11:50	**IL: Matthew Bone,** Bristol Composites Institute, University of Bristol, University Walk, Bristol, UK High Throughput Modelling of Polymers with Molecular Dynamics and Machine Learning
	12:20	**IC: Froze Jameel,** Max Planck Institute for Dynamics of Complex Technical Systems, Germany Solvent Design for Green Homogeneous multi-phase Industrial Reactions
	12:40	**IC: Parvathi Krishnakumar,** University of Limerick, Ireland Predicting Thermodynamic Properties of Novel Compounds from their Starting Materials
13:00-14:30	**Poster Session II**	
13:00-14:30	**Lunch**	
14:30-16:30	**Discovering Thessaloniki** **Board Meeting, EuChemS Division of Computational and Theoretical Chemistry** (Seminar Hall, Olympic Museum of Thessaloniki)	
16:30 -17:50	**Materials Design** Chair: **Mercè Deumal**	
	16:30	**IC: Colm Burke,** University of Liverpool, UK High-throughput atomistic modelling of semiconducting polymers
	16:50	**IC: Irene Casademont Reig,** Vrije Universiteit Brussel, Belgium Manipulating Excited Estates using Inverse Design
	17:10	**IC: Julian Holland,** University of Southampton, UK Modelling LLZO: Limiting Structures in a Near-unlimited Configuration Space
	17:30	**IC: Ioannis Skarmoutsos,** University of Ioannina, Greece The unique structural features of water, ranging from ambient liquid up to supercritical, extreme-pressure conditions: Insights from classical and ab initio molecular dynamics simulations

Invited Contribution: **IC** | Invited Lecture: **IL** | Keynote Lecture: **KL** | Short Communication: **SC**

17:50-18:00	**Short Break**	
18:00-19:05	**Short Communications** Chair: **Stefan Kast**	
	Biomolecular Systems	
	18:00	**SC: Charlotte Bouquiaux,** University of Namur, Belgium Investigating the influence of the lipid structure on the global membrane organization: effect of the fatty acids
	18:05	**SC: Ho Ting Henry,** University of Oxford, UK Substrate Binding Dynamics of SARS-CoV-2 Cysteine Proteases
	18:10	**SC: Gianmarco Lazzeri,** Frankfurt Institute for Advanced Studies, Germany Reconstructing Rare Event Kinetics Using AI-enhanced Unbiased Molecular Dynamics Simulations
	18:15	**SC: Carlos Sequeiros-Borja,** Adam Mickiewicz University, Poland Water will find a way: transport through narrow tunnels and its significance in enzymes
	18:20	**SC: Andrea Levy,** École Polytechnique Fédérale de Lausanne (EPFL), Switzerland Addressing Challenges in Computational Simulations of Covalently Binding Transition Metal-Based Drugs
	Artificial Intelligence in Chemical Research	
	18:25	**SC: Hannes Kneiding,** University of Oslo, Norway Machine Learning Quantum Properties of Transition Metal Complexes with Natural Quantum Graphs
	18:30	**SC: Elliot Farrar,** University of Bath, UK Machine learning and semi-empirical calculations: A synergistic approach to rapid, accurate, and mechanism-based reaction barrier prediction
	18:35	**SC: Edoardo Cignoni,** University of Pisa, Department of Chemistry and Industrial Chemistry, Italy Machine Learning Exciton Hamiltonians in Light-Harvesting Complexes
	18:40	**SC: Frédéric Celerse,** École Polytechnique Fédérale de Lausanne (EPFL), Switzerland Machine learning potentials for simulating solvent-assisted reactions
	18:45	**SC: Eugen Hruška,** Charles University, Czech Republic Bridging the explicit solvation experiment-calculation divide with machine learning and high-throughput simulation
	Materials Design	
	18:50	**SC: Edoardo Donadoni,** University of Milano-Bicocca, Italy Multi-scale modeling of folic acid-functionalized TiO_2 nanoparticles for active targeting of tumor cells
19:05-20:30	**Poster Session III**	

08:45-10:45	**Biomolecular Systems** Chair: **Michael Otyepka**	
	08:45	**KL: William Jorgensen,** Department of Chemistry, Yale University, USA Evolution of Free-Energy Calculations
	09:30	**IL: Kennie Merz,** Michigan State University, USA Molecular Gas Phase Conformational Ensembles
	10:00	**IC: Danai Maria Kotzampasi,** Biomedical Research Foundation Academy of Athens, Greece Insights into the mechanism of the C-terminal PIK3CA activating mutations
	10:15	**IL: Klaus Liedl,** University of Innsbruck, Austria Antibody Structure and Dynamics in Solution
10:45 - 11:15	**Coffee | Tea Break**	
11:15-13:15	**Biomolecular Systems** Chair: **Zoe Cournia**	
	11:15	**IL: Marco de Vivo,** Istituto Italiano di Tecnologia, Italy Function and inhibition of cation-coupled chloride cotransporters
	11:45	**IL: Chris Oostenbrink,** University of Natural Resources and Life Sciences, Vienna, Austria Free energies and enhanced sampling from accelerated enveloping distribution sampling
	12:15	**IC: Tobias Hüfner,** Max-Planck Institute for Biophysics, Germany Automated and Systematic Derivati on of Parameter Type Definitions for Molecular Mechanics Force Fields
	12:35	**IC: Katie Kuo,** Georgia Institute of Technology, USA From Closed to Open: Addressing the Role of the Efflux Pump AcrAB-TolC in Antibiotic Resistance
	12:55	**IC: Dan Major,** Bar-Ilan University, Israel Screening Enzyme Mechanisms using Multiscale Mechanistic Docking with EnzyDock
13:15-14:30	**Lunch**	
14:30-16:25	**Artificial Intelligence in Chemical Research** Chair: **Tanja Van Mourik**	
	14.30	**KL: Edward Pyzer-Knapp,** IBM Research-Europe, UK How AI accelerates the discovery of new molecules and materials
	15.15	**IL: Ganna Gryn'ova,** Heidelberg Institute for Theoretical Studies, Germany New representations for interpretable chemical machine learning
	15.45	**IC: Amol Thakkar,** IBM Research Europe, Switzerland Multi-Cloud Data Infrastructure for AI Foundation Models in Chemical Research
	16.05	**IC: Paul Katzberger,** ETH Zürich, Switzerland Graph Neural Networks as Implicit Solvents in MD Simulations
16:25-17:00	**Coffee | Tea Break**	

17:00-18:20	**Artificial Intelligence in Chemical Research** Chair: **Antti Poso**	
	17:00	**IC: Veronika Juraskova,** University of Oxford, UK Modelling Chemical Processes in Explicit Solvents with Machine Learning Potentials
	17:20	**IC: Elin Dypvik Sødahl,** Norwegian University of Life Sciences, Norway Investigating molecular rotations in ferroelectric plastic crystals using machine learned force fields
	14:40	**IC: Marco Bortoli,** University of Oslo, Norway Development of Machine Learning Potentials for Main Group Organometallic Reagents
	18:00	**IC: Massimo Delle Piane,** Politecnico di Torino, Italy Machine Learning Approaches to Unravel the Dynamic Behavior of Metal Surfaces and Nanoparticles
18:40-20:00	**Poster Session IV**	
20:00-21:00	**Break**	
21:00	**Conference Dinner (Makedonia Palace Hotel, 2. M. Alexandrou Av)**	

08:40-10:20	**Biomolecular Systems** Chair: **Ivelina Georgieva**	
	08.40	**IC: Joep Wals,** University of Antwerp, Belgium Molecular Dynamics Simulations on UAMC-0001305 Warhead Derivatives to Theragnostically Target Fibroblast Activation Protein
	09.00	**IC: Stefano Serapian,** University of Pavia, Italy Learning the Languages of Allostery in K-Ras4B
	09.20	**IC: Dhiman Ray,** Italian Institute of Technology, Italy Data-Driven Classification of Ligand Unbinding Pathways and Kinetics
	09.40	**IC: Anastasia Rissanou,** National Hellenic Research Foundation, Greece A Computational Study of the Complexation of Single Stranded RNA with Lipid-based Agents
	10.00	**IC: Francesco Saverio di Leva,** University of Naples Federico II, Italy Free Energy Calculations in the Revival of Old-but-New Therapeutic Targets: Discovery and Development of RGD Integrin Peptides
10:20-10:50	**Coffee | Tea Break**	
10:50-12:10	**Biomolecular Systems** Chair: **Safiye Erdem**	
	10:50	**IC: Peter Starrs,** University of St Andrews, UK Molecular Dynamics Study of Arabinoxylan Polymer Flexibility with Forcefield Comparison
	11:10	**IC: Marketa Paloncyova,** Palacky University Olomouc, Czech Republic Lipid Nanoparticles: From Structure to Interactions with Cell Membranes
	11:30	**IC: Matteo Capone,** University of L'Aquila, Italy Alternative Fast and Slow Primary Charge-Separation Pathways in Photosystem II
	11:50	**IC: Vassilios Myrianthopoulos,** National and Kapodistrian University of Athens, Greece Right tools for the job. Simple and sophisticated approaches for enhancing performance of in silico methodologies in drug discovery
12:10-13:10	**Electronic Structure: Theory and Applications** Chair: **Peter Reinhardt**	
	12:10	**IC: Bernardo de Souza,** FAccTs GmbH, Germany On the importance of conformational Entropy when predicting Chemistry: results from the new Global Optimizer AlgoriThm (GOAT) implemented in ORCA
	12:30	**IC: Mario Piris,** DIPC & EHU/UPV & IKERBASQUE, Spain Time evolution of natural orbitals in ab initio molecular dynamics
	12:50	**IC: Adriana Pecoraro,** University of Naples Federico, Italy First-principles prediction of exotic hexagonal NaCl films on methylammonium lead iodide substrates, new hints for perovskite solar cells
13:10-14:30	**Lunch**	

14:30-15:50	**Electronic Structure: Theory and Applications** Chair: **Péter G. Szalay**	
	14:30	**IC: Yannik Schütze,** Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany Multiscale modeling of conjugated organosulfur polymer cathodes for lithium-sulfur batteries
	14:50	**IC: Aslihan Sumer,** Saglik Bilimleri Universitesi, Turkey CO Oxidation on Molybdenum Oxide Clusters: Reaction Energetics and Mechanism
	15:10	**IC: Marc de Wergifosse,** Université Catholique de Louvain, Belgium The eXact integral simplified time-dependent density functional theory (XsTD-DFT)
	15:30	**IC: Örs Legeza,** Wigner Research Centre for Physics, Hungary Predicting the FCI energy of large systems to chemical accuracy from restricted active space density matrix renormalization group calculations via Hybrid CPU-GPU based architectures
15:50	**Awards | Farewell**	
16:30	**End of Conference**	
18:30-23:00	**Optional visit to the Museum of Byzantine Culture, Thessaloniki (free entrance)**	

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