e-EuCo-CTC 2021

Online conference
EuChemS Division of
Computational and Theoretical Chemistry

November 18-19 2021, 2-7pm CET

European Conference in Theoritical and Computational Chemistry
CONFERENCE PROGRAMME

Organizing and Scientific Committee
Zoe Cournia
Hans Peter Lüthi
Benoît Champagne
Mercè Deumal
Stefan M. Kast
Tanja van Mourik
Katarina Nikolić
Ivelina Georgieva
Radu Silaghi-Dumitrescu
Péter G. Szalay

Sessions

- Artificial Intelligence in Chemical Research
- Materials
- Biomolecular Systems
- Electronic Structure

All times are CET times

Talk Duration

Invited talks : 30 minutes (25 + 5)

Short talks: 20 minutes (15 + 5)

Flash talks: 3 minutes

Thursday, 18 November		
Time (CET)	**Speaker**	**Title**
14:00	**Zoe Cournia**, Biomedical Research Foundation, Academy of Athens, Greece, Conference Chair **Hans Peter Luethi**, ETH Zürich and Swiss Chemical Society, Switzerland, Conference co-Chair	Opening Remarks & Logistics
14:10	**Peter Szalay**, President of the Division of Theoretical and Computational Chemistry, EuChemS and Eötvös University, Hungary	Overview of the EuChemS Computational and Theoretical (CTC) Division
Artificial Intelligence in Chemical Research **Chair: Benoît Champagne**		
14.15	**Keynote Speaker:** **Teodoro Laino**, IBM, Switzerland	The Power of Language in Chemistry (and more)
14.45	**Leticia Manén Freixa**, Universitat Ramon Llull, Spain	Exploring Molecular Diversity in Drug Discovery: There is Plenty of Room at Markush's
15.05	**Theodorus P.M. Goumans**, Software for Chemistry & Materials, the Netherlands	Accelerated Materials Innovation Through Machine-Learning Assisted Atomistic Modeling

15.25	**Alexios Chatzigoulas**, Biomedical Research Foundation, Academy of Athens, Greece	Predicting protein-membrane interfaces of peripheral membrane proteins using ensemble machine learning
15.45	Coffee Break, Award Voting, Sponsor Presentation	
Materials **Chair: Tanja van Mourik**		
16.00	**Keynote Speaker:** **Nong Artrith,** Utrecht University, the Netherlands	Modelling of Complex Energy Materials with Machine Learning
16.30	**Adriana Pietropaolo**, Università di Catanzaro, Italy	Multi-replica biased sampling for photoswitchable conjugated frameworks
16.50	**Daniel Reta**, Euskal Herriko Unibertsitatea and Donostia International Physics Center, Spain	Ab initio spin dynamics of high-performing single molecule magnets
17.10	**Camille Latouche**, CNRS, Institut des Matériaux Jean Rouxel, Université de Nantes, France	Modelling excited states in solids: ZrO2:Ti and Scapolite as test cases
17.30	Coffee Break, Award Voting, Sponsor Presentation	
Flash Presentations – Artificial Intelligence in Chemical Research **Chair: Hans Peter Lüthi**		
17.40	**Raúl Pérez-Soto**, Institute of Chemical Research of Catalonia, Spain	Benchmarking clustering algorithms for macrocyclic conformational sampling
17.44	**Siddharth S. Ghule,** CSIR-National Chemical Laboratory, India	Predicting the Redox Potentials of Phenazine Derivatives using DFT Assisted Machine Learning
17.48	**Ramon A Miranda Quintana**, University of Florida, USA	Tackling Big Data problems in chemistry with extended similarity indices

17.52	**Endika Torres**, Instituto Quimíco de Sarriá, Spain	Design and synthesis of multitarget Tyrosine Kinase Inhibitors for pancreatic cancer
17.55	Short Break	
Flash Presentations – Materials **Chair: Mercè Deumal**		
18.00	**Yannik Schütze,** Helmholtz Zentrum Berlin für Materialien und Energie, Germany	Combined first principles-statistical mechanics approach to sulfur structure in organic cathode hosts for polymer based lithium-sulfur (Li-S) batteries
18.04	**Estefanía Díaz López**, Universitat Autònoma de Barcelona, Spain	CO2 hydrogenation to methanol led by the Cu-Mo2C interface
18.08	**Kalishankar Bhattacharyya**, Max-Planck-Institut für Kohlenforschung, Germany	Structure and Reactivity of IrOx Nanoparticles for the Oxygen Evolution Reaction in Electrocatalysis: An Electronic Structure Theory Study
18.12	**Manuel J Kolb**, University of Barcelona IQTC, Spain	Structure Sensitive Scaling Relations among Carbon-Containing Species
18.16	**Saeed Amirjalayer**, University of Münster, Germany	On the cooperative interplay of molecular machines embedded in functional materials
18.20	**Jordi Poater**, Universitat de Barcelona, Spain	Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications
18.25	Short Break	
Flash Presentations – Biomolecular Systems **Chair: Zoe Cournia**		
18.30	**Cristian Privat Contreras**, University of Barcelona, Spain	Deciphering Constant pH Molecular Dynamics in Short Peptides
18.34	**Giacomo Salvadori**, University of Pisa, Italy	On the photoactivation of a bacteriophytochrome through a QM/MM Surface Hopping approach

18.38	**Marcel Bermudez**, University of Münster, Germany	A dynamic view on receptor-ligand interactions
18.42	**Oksana Azpitarte**, University of the Basque Country, Spain	Structural and conformational study of FMN-containing miniSOG
18.46	**Liadys Mora Lagares**, National Institute of Chemistry Theory Department, Slovenia	Structure-Function Relationships in the Human P-glycoprotein (ABCB1): Insights from Molecular Dynamics Simulations
18.50	**Jose Y. Kaneti**, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgaria	Large Scale DFT and Explicitly Correlated MO Computations on Guanine Quadruplexes and their Heterocyclic Adducts
18.54	**Sofia Slavova**, Bulgarian Academy of Sciences	A theoretical study of pyrimidine nucleobases formation from formamide
End of first day		

Friday, 19 November		
Time (CET)	**Speaker**	**Title**
14:00	**Zoe Cournia**, Biomedical Research Foundation, Academy of Athens, Greece, Chair **Hans Peter Luethi**, ETH Zürich and Swiss Chemical Society, Switzerland, co-Chair	Opening Remarks & Logistics
Biomolecular Systems **Chair: Zoe Cournia**		
14.10	**Keynote Speaker:** **Stefan Güssregen**, Sanofi-Aventis, GmbH, Germany	Automated Design of Macrocycles for Therapeutic Applications
14.40	**Markéta Paloncýová**, Czech Advanced Technology and Research Institute, Czech Republic	Lipids in SARS-CoV-2 Vaccines: From Membrane Structure to Interaction with mRNA Fragments
15.00	**Birgit Strodel**, Forschungszentrum Jülich, Germany	Effects of in vivo conditions on peptide aggregation: computational approaches
15.20	**Pedro Fernandes**, University of Porto, Portugal	Fine details of the pre-organization of enzyme active sites and their role in enzyme catalysis and engineering
15.40	**Katarina Nikolić**, University of Belgrade, Serbia	Epigenetic drug discovery: Successful examples of Computer-Aided Drug Designing of Histone Deacetylase (HDAC6 and SIRT2) and Histone Methyltransferase (DOT1L) inhibitors
16.00	Coffee Break, Award Voting, Sponsor Presentation	

Electronic Structure **Chair: Ivelina Georgieva**		
16.15	**Keynote Speaker:** **Markus Reiher**, ETH Zürich, Switzerland	From Electronic and Vibrational Structure to Quantum Dynamics with Matrix Product States
16.45	**Boris Maryasin**, University of Vienna, Austria	Computationally Driven Organic Chemistry: Making Theory Practical
17.05	**Anna Hehn**, University of Zurich, Switzerland	Increasing efficiency for theoretical absorption and emission spectroscopy of extended systems
17.25	**Daniel Escudero,** Katholieke Universiteit te Leuven, Belgium	Benchmarking excited state decay rate calculations
17.45	Coffee Break, Award Voting, Sponsor Presentation	
Flash Presentations – Biomolecular Systems **Chair: Stefan Kast**		
18.00	**Nicolas Chéron**, CNRS & Ecole Normale Supérieure, France	Binding site of bicarbonate in PEP Carboxylase
18.04	**Charlotte Bouquiaux**, University of Namur, Belgium	Multiscale Theoretical Investigation of the Second Harmonic Generation of Di-8-ANEPPS in (Un)Saturated Lipid Bilayers: Effect of the Cholesterol Content
18.08	**Pierre Beaujean**, University of Namur, Belgium	All-Atom Quantum Mechanical Calculation of the Second-Harmonic Generation of Fluorescent Proteins
18.12	**Maria G. Khrenova,** Lomonosov Moscow State University, Russia	Mechanistic and electronic structure aspects of the N-acetyl-L-aspartyl-L-glutamate hydrolysis by glutamate carboxypeptidase
18.16	**Sergey Katsyuba**, A.E. Arbuzov Institute of Organic and Physical Chemistry, Russia	How to Simulate Infrared Spectra of Conformationally Flexible Molecules in Liquids and in Hydrogen-Bonded Solvents

18.20	**Goedele Roos**, Université de Lille, France	Histidine versus cysteine bearing heme-dependent halogen peroxidases: parallels and differences for Cl- oxidation
18.24	**Shaima Hashem**, University of Pisa, Italy	From crystallographic data to the solution structure of photoreceptors: the case of the AppA BLUF domain
18.28	**Isabelle Navizet,** Université Gustave Eiffel, France	QM/MM studies of bioluminescent systems
18.32	Short Break	
Flash Presentations – Electronic Structure **Chair: Péter Szalay**		
18.40	**Sergei F. Vyboishchikov,** University of Girona, Spain	Fast non-iterative calculation of solvation energies of molecules and ions
18.44	**Carlos M. R. Rocha,** Leiden University, the Netherlands	Pushing the boundaries of electronic structure theory: theoretical spectroscopic characterization of small interstellar anions – the case of C2N-
18.48	**Stefano Evangelisti,** Université Toulouse III, France	Clifford Boundary Conditions for Periodic Systems
19.52	**Kati Finzel,** Technische Universität Dresden, Germany	The bifunctional formalism – An alternative treatment of density functionals
19.56	**Coen de Graaf**, University Rovira i Virgili, Spain	Intermolecular energy and electron transfer through non-orthogonal configuration interaction
19.00	**Silvia Escayola**, University of Girona, Spain	Tuning the Aromaticity of Excited para-quinodimethanes
19.05	**Concluding Remarks**	
End of conference		