Monday 13th July 2026
Congress theme:
Computational Chemistry & AI The Power of Data

Session	Timing	Presenter	Title
1	10:00-10:15	Irina Grubova	Binding Energies of Sulfur–Bearing Species on Neutral and Charged Amorphous Solid Water Ices
2	10:15-10:30	tbd	
3	10:30-10:45	Carles Bo	New Computational Insights into the Speciation and Formation of Polyoxometalates
4	10:45-11:00	Shang-Hao Chiang	DFT Insights into GaSe/InS Heterostructures for Visiblef-Light-Driven Water Splitting with High Solar-to-hydrogen Efficiency
5	11:00-11:15	Carlo Alberto Gaggioli	Modelling Singlet Oxygen Generation on Ru-functionalized Metal Organic Frameworks with Trapped Ion Quantum Computers
6	11:15-11:30	Feixiang Xu	Multiscale Computational Insights into Thermal and Catalytic Pyrolysis of Polyolefins
7	11:30-11:45	Elisabetta Inico	Carbonate-Radical Pathway in Dual Nickel/Carbon Nitride Photocatalysis: A New Mechanistic Blueprint for C(sp3)-H Activation
8	11:45-12:00	Yuman	PyOrbb — Automated Analysis Tool for Orbital Interactions
Invited lecture	14:00-14:30	**Maria Ramos**	Computational Enzymology and AI
3	14:30-14:45	Carlo Alberto Gaggioli	Molecular aggregation and Microheterogeneity in various aqueous solutions
4	14:45-15:00	Przemysław Grenda	CYtochrome Complex Ligand Optimization with Protein Simulation – an automated pipeline for simulations and analysis of CYP450 docked structures
5	15:00-15:15	Ioana M. Ilie	Computational engineering of peptides inhibiting cell death
6	15:15-15-30	Kenno Vanommeslaeghe	The Sampling-based Adaptive Biasing Force (sABF) method efficiently explores the free energy landscape of large-scale motions in liquid-phase systems
7	15:30-15:45	Eugen Hruška	Higher accuracy reaction rates with the ab initio nanoreactor
8	15:45-16:00	Christophe de Graaf	Bridging molecular dynamics and COSMO-RS simulations with macroscale modeling for advancements in Polyurethane post depolymerization separation processes
1	16:30-16:45	Anna Bondarenko	Modeling charge transport in radical-containing polymers for all-organic batteries
2	16:45-17:00	Ionut Tranca	Catch the Heat : in Porous and Non-porous Materials
3	17:00-17:15	Andrew Tarzia	Unbiased structure prediction of molecular cages
4	17:15-17:30	Lorenzo Baldinelli	Harnessing Noncovalent Interactions from Catalysis to Quantum Technologies
5	17:30-17:45	Maxim Papusha	StereoMolGraph: Reliable Computational Toolkit for Chiral Molecules and Reactions
6	17:45-18:00	Ivan Kodrin	Computationally assisted analysis of CO2 adsorption in nitrogen-nitrogen linked porous organic polymers

Tuesday 14th July 2026
Congress theme:
Computational Chemistry & AI The Power of Data

Session	Timing	Presenter	Title
1	10:00-10:15	Martijn Hut	Training of Machine-learned Force Fields for Modeling Metal–Support Interactions in Catalysis
2	10:15-10:30	Gregor Simm	SimPoly: Simulation of Polymers with Machine Learning Force Fields Derived from First Principles
3	10:30-10:45	Elpiniki Paspali	AI-driven generative and rational design of peptide modulators targeting GUCY2C for Parkinson's disease
4	10:45-11:00	Philippa Cox	Computationally driven exploration of the structure and electronic properties of Cu2GeSe3 for use in high-performance thin film photovoltaic alloys
5	11:00-11:15	Robbe Devreese	Collisional cross-section prediction of peptides and small molecules: covering all bases and bridging the gap
6	11:15-11:30	Jelle Vekeman	Machine Learning Potentials at Speeds Comparable to Reactive Force Fields
7	11:30-11:45	tbd	
8	11:45-12:00	Mohammed Bin Jassar	Packed by the Surface: Relating Surface Structure and Solvation Properties at Solid/Water Interfaces
Invited lecture	14:00-14:30	**Phillip Schwaller**	Accelerating Chemical Science in the Era of LLMs
3	14:30-14:45	Krishna Govender	Chemoinformatics profiling of Annona muricata-derived compounds targeting COX-2 in breast cancer
4	14:45-15:00	Alexander Messler	Uncertainty-aware prediction of 195Pt chemical shifts from limited data
5	15:00-15:15	Muhammad Umer	Machine learning force fields for accelerated design and discovery of electrocathodic materials
6	15:15-15-30	Paul Popelier	FFLUX: Machine Learnt Potentials based on Quantum Topological Atoms
7	15:30-15:45	Sergey Varnavskiy	Data-centric AI in computational chemistry: integrating curated literature with other data
8	15:45-16:00	Trung Trinh	Data-Driven Process Intensification of Methyl Acetate Production via Surrogate-Based Bayesian Optimization
1	16:30-16:45	Elham Sattarinezhad	Exploring the Mechanism of Protochlorophyllide to Chlorophyllide Conversion
2	16:45-17:00	Fardine Ameli	Replica Exchange with Flexible Timing (REFT): a novel replica exchange variant for efficient conformational sampling and free energy calculations
3	17:00-17:15	Hilal Kalkan	Computational Screening of Triphenylamine-Based Star-Shaped Molecules: Insights into Electronic and Optical Properties for Organic Photovoltaic
4	17:15-17:30	Steven Beutick	Lone-Pair Shielded Radicals: Beyond the Captodative Substitution Pattern
5	17:30-17:45	Giovanni Bistoni	Novel computational strategies for the study of chemical selectivity: Combining high accuracy and chemical insight
6	17:45-18:00	Christoph Plett	ORCA Meets Python – The ORCA Python Interface OPI

Wednesday 15th July 2026
Congress theme:
Computational Chemistry & AI The Power of Data

Session	Timing	Presenter	Title
1	10:00-10:15	Simen Camps	Resolving spin contamination in spin-flip methods: the extended spin-flip CC2 method
2	10:15-10:30	Hans Lischka	Machine learning and multireference configuration interaction for high-level nonadiabatic dynamics simulation of hexatriene
3	10:30-10:45	Tommaso Giovannini	Driving Chemistry through Plasmonic Photoinduced Phenomena: An Atomistic Perspective
4	10:45-11:00	Federico Rossi	Convex Hartree-Fock and Density Functional Theory for Stable Simulations at Conical Intersections
5	11:00-11:15	Federica Borzelli	Computational modeling of tryptophan fluorescence spectra in proteins
6	11:15-11:30	Francesco Di Maiolo	Organic Diradicals Bridged by Inverted Singlet-Triplet Units for Optical-Spin Interfaces
7	11:30-11:45	Jordi Cirera	Data-Driven Prediction of Spin-Crossover Properties from Electronic Structure Calculations
8	11:45-12:00	Jasper Schuurmans	Digital twins to design reactors for efficient photochemistry
Invited lecture	14:00-14:30	**Rigoberto Hernandez**	
3	14:30-14:45	Ji Liu	Formation of oxynitrides under ambient condition during post-deposition process: an ab initio molecular dynamics study on the oxidation process of metal nitrides
4	14:45-15:00	Hsin-Yi Tiffany Chen	Multiscale modeling of hydrogen coverage on Ru nanoparticle: a combined DFT, AIMD, and DPMD study
5	15:00-15:15	Edoardo Panzetta	Computational study of N-methylacetamide (NMA) amide bond cleavage reaction in neutral and alkaline conditions
6	15:15-15-30	Giulia Ciattaglia	A computational study of beta cyclodextrin-based nanosponge inclusion complexes
7	15:30-15:45	Torsten John	From Mechanisms to Function: Computational Studies of Peptide Self-Assembly at Interfaces
8	15:45-16:00	Horacio Poblete	Programmable Peptide–Graphite Interfaces for Water Bioremediation: From Gly–X Sequence to Ion Capture
1	16:30-16:45	Silvia Casassa	CRYSTAL, an ongoing project for a theoretical chemical approach to solids
2	16:45-17:00	Marta Corno	Multiscale approaches to drug encapsulation and release in β-cyclodextrin-based systems
3	17:00-17:15	Bónis Barcza	Including charge transfer states in fragment based exciton calculations
4	17:15-17:30	Filippo Sacchetta	Efficient Low-Scaling Calculation of THC-SOS-LR-CC2 and THC-SOS-ADC(2) Excitation Energies Through Density-Based Integral-Direct Tensor Hypercontraction
5	17:30-17:45	Thomas Jagau	Recent progress in computational Auger spectroscopy
6	17:45-18:00	Alistair Sterling	Seamless integration of machine-learned interatomic potentials into quantum chemistry workflows with ChemRefine

Thursday 16th July 2026
Congress theme:
Computational Chemistry & AI The Power of Data

Session	Timing	Presenter	Title
1	10:00-10:15	tbd	
2	10:15-10:30	Zhaochun Liu	A machine-learning–driven multiscale investigation of low-cost thermochemical heat storage materials based on LiCl–LiBr solid solutions
3	10:30-10:45	Jorge J. Carbó	3D-QTAIM Descriptor-Based Modeling for Asymmetric Catalysis
4	10:45-11:00	Cheng-Chung Wang	AI and statistical analysis for understanding stereoselective glycosylation reactions
5	11:00-11:15	Laura Falivene	Chiral Deep Eutectic Solvents as Catalysts for Asymmetric Synthesis: A Machine Learning–Driven Molecular Dynamics Design Tool
6	11:15-11:30	Tobe Vorsselmans	Water and CO Desorption from Amorphous Carbon Surfaces: A Computational and Experimental Study
7	11:30-11:45	Yongsheng Huang	Multi-Scale Investigation Of Triboelectric Nanogenerator: An Expanded DFT Calculation Based on Machine Learning
8	11:45-12:00	Joep Wals	Binding mechanism of UAMC-1110 to Fibroblast Activation Protein
Invited lecture	14:00-14:30	**Francoise Remacle**	Tentative title: Control of molecular reactivity with attopulses
3	14:30-14:45	Marilù Maraldi	Realistic simulations of nonlinear optical photoswitches with novel all-atom quantum mechanical methodologies
4	14:45-15:00	Markus Weiss	Asymmetrically-constrained Adiabatic ALMO-EDA: Designing Catalysts from First Principles
5	15:00-15:15	Florian Matz	All correlation within a mean field: Assessment of i-DMFT and the modified Collins conjecture
6	15:15-15:30	Francesco Calcagno	Quantum Chemistry Is All You Need: Data-free Inverse Molecular Design with PROTEUS