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

Session	Timing	Presenter	Title
CAI - D1 - O1	10:00-10:15	Irina Grubova	Binding Energies of Sulfur–Bearing Species on Neutral and Charged Amorphous Solid Water Ices
CAI - D1 - O2	10:15-10:30	Ramadhan Muhammad Dzulfahmi	Uncovering the origin of amine-driven selectivitiy in Ru-catalyzed CO2-to-methanol hydrogenation
CAI - D1 - O3	10:30-10:45	Carles Bo	New Computational Insights into the Speciation and Formation of Polyoxometalates
CAI - D1 - O4	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
CAI - D1 - O5	11:00-11:15	Carlo Alberto Gaggioli	Modelling Singlet Oxygen Generation on Ru-functionalized Metal Organic Frameworks with Trapped Ion Quantum Computers
CAI - D1 - O6	11:15-11:30	Feixiang Xu	Multiscale Computational Insights into Thermal and Catalytic Pyrolysis of Polyolefins
CAI - D1 - O7	11:30-11:45	Elisabetta Inico	Carbonate-Radical Pathway in Dual Nickel/Carbon Nitride Photocatalysis: A New Mechanistic Blueprint for C(sp3)-H Activation
CAI - D1 - O8	11:45-12:00	Yuman	PyOrbb — Automated Analysis Tool for Orbital Interactions
POSTER FLASH	12:00		
CAI - D1 - F01		Jeloadre Kvan	A Closed-loop and Self-driving Precision Polymer Synthesis Platform Using ML
CAI - D1 - F02		Calero Mendoza Rolando	DFT–QSAR Integrated Modeling of Betanin-Derived Green Corrosion Inhibitors for Reinforced Concrete in Marine Environments
CAI - D1 - F03		Brea Oriana	Impact of Fast Mechanistic Studies in Industrial Setting
CAI - D1 - F04		Baets Peter	Addressing process challenges through AI: Biobased amine production in flexizyme
CAI - D1 - F05			
CAI - D1 - F06		Badida Wissal	Deep Learning–Driven In Silico Analysis of Cannabis Phytocannabinoids for Therapeutic Discovery
CAI - D1 - F07		Kumari Geetu	In silico Engineering of Piezoelectric Biomolecular Assemblies
Lunch			
CAI - D1 - I1	14:00-14:30	**Maria Ramos**	Computational Enzymology and AI
CAI - D1 - O9	14:30-14:45	Carlo Alberto Gaggioli	Molecular aggregation and Microheterogeneity in various aqueous solutions
CAI - D1 - O10	14:45-15:00	Przemysław Grenda	CYtochrome Complex Ligand Optimization with Protein Simulation – an automated pipeline for simulations and analysis of CYP450 docked structures
CAI - D1 - O11	15:00-15:15	Ioana M. Ilie	Computational engineering of peptides inhibiting cell death
CAI - D1 - O12	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
CAI - D1 - O13	15:30-15:45	Eugen Hruška	Higher accuracy reaction rates with the ab initio nanoreactor

CAI - D1 - O14	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
Coffee break			
CAI - D1 - O15	16:30-16:45	Anna Bondarenko	Modeling charge transport in radical-containing polymers for all-organic batteries
CAI - D1 - O16	16:45-17:00	Ionut Tranca	Catch the Heat : in Porous and Non-porous Materials
CAI - D1 - O17	17:00-17:15	Andrew Tarzia	Unbiased structure prediction of molecular cages
CAI - D1 - O18	17:15-17:30	Lorenzo Baldinelli	Harnessing Noncovalent Interactions from Catalysis to Quantum Technologies
CAI - D1 - O19	17:30-17:45	Maxim Papusha	StereoMolGraph: Reliable Computational Toolkit for Chiral Molecules and Reactions
CAI - D1 - O20	17:45-18:00	Ivan Kodrin	Computationally assisted analysis of CO2 adsorption in nitrogen-nitrogen linked porous organic polymers
Posters			
CAI - D1 - P01		Asghar Basim	Thiazole Schiff Bases as Molecular Shields for Mild Steel: Novel Insights from Experimental and Computational Investigations
CAI - D1 - P02		Chandrasekar Aditi	Synergistic Hydrogen-Bonding and CO2 Activation: A Sustainable Metal, Halogen, and Solvent-Free Strategy
CAI - D1 - P03		Damayanti Krista	Machine learning prediction for polymer glass transition temperature with SHAP interpretation
CAI - D1 - P04		Sheu Sheh-Yi	High-Performance Energy-Free Desalination
CAI - D1 - P05		Sigmund Lukas	BONAFIDE: A Python Package for Calculating Features for Atoms and Bonds in Molecules
CAI - D1 - P06		Motmans Brent	Predictive inorganic synthesis from small data using machine learning: size-controlled Cu nanoparticles
CAI - D1 - P07		Ganesan Krithika	Defect mediated surface modification of amorphous TiO2 surface using Grignard reagent in explicit solvation model
CAI - D1 - P08		Odai Kei	Theoretical study of the interaction between 3α-hydroxysteroid dehydrogenase and androsterone
CAI - D1 - P09		Rodríguez Fileto	Understanding the Raman Spectra of Silica Prenucleation Clusters via Ab Initio Molecular Dynamics and Experiments
CAI - D1 - P10		Hobbs Christopher	Chemical Accuracy in Computational Prediction of PFAS-Cyclodextrin Binding: A Multi-Level SQM/QM Study with Experimental ITC Validation

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

Session	Timing	Presenter	Title
CAI - D2 - O1	10:00-10:15	Martijn Hut	Training of Machine-learned Force Fields for Modeling Metal–Support Interactions in Catalysis
CAI - D2 - O2	10:15-10:30	Gregor Simm	SimPoly: Simulation of Polymers with Machine Learning Force Fields Derived from First Principles
CAI - D2 - O3	10:30-10:45	Elpiniki Paspali	AI-driven generative and rational design of peptide modulators targeting GUCY2C for Parkinson's disease
CAI - D2 - O4	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
CAI - D2 - O5	11:00-11:15	Robbe Devreese	Collisional cross-section prediction of peptides and small molecules: covering all bases and bridging the gap
CAI - D2 - O6	11:15-11:30	Jelle Vekeman	Machine Learning Potentials at Speeds Comparable to Reactive Force Fields
CAI - D2 - O7	11:30-11:45	Francesco Calcagno	Quantum Chemistry Is All You Need: Data-free Inverse Molecular Design with PROTEUS
CAI - D2 - O8	11:45-12:00	Mohammed Bin Jassar	Packed by the Surface: Relating Surface Structure and Solvation Properties at Solid/Water Interfaces
POSTER FLASH	12:00		
CAI - D2 - F01		Naumkin Fedor	Towards molecular iontronics: Intra-complex "through" vs "around" ion transfer
CAI - D2 - F02		Ekmekci Cumhur Gokhan	Structure-based discovery of NLRP3 inflammasome inhibitors: an integrated computational approach combining virtual screening, molecular dynamics, and binding free energy calculations
CAI - D2 - F03		Ekmekci Cumhur Gokhan	Structure-based identification of novel USP7 inhibitors targeting the p53-MDM2 axis: a computational approach for anticancer drug discovery
CAI - D2 - F04		Leherte Laurence	Mimicking the effect of displacement parameter and crystallographic resolution on the topology of electron density distributions: application to non-covalent interactions
CAI - D2 - F05		Lipin Raju	How Subsurface Carbon Affects Hydrogen Interactions at Transition Metal Electrodes
CAI - D2 - F06		Hruška Eugen	Bridging chemical property explainability between chemistry and machine learning
CAI - D2 - F07		Stany Lionel Tsomene Doungmo	Harnessing natural flavonoids and biflavonoids from a Cameroonian plant roots for Neuroprotection and Depression Therapy: Integrative Spectroscopic, Computational and Pharmacological Approaches
Lunch			
CAI - D3 - I1	14:00-14:30	**Phillip Schwaller**	Accelerating Chemical Science in the Era of LLMs
CAI - D2 - O9	14:30-14:45	Krishna Govender	Chemoinformatics profiling of Annona muricata-derived compounds targeting COX-2 in breast cancer
CAI - D2 - O10	14:45-15:00	Alexander Messler	Uncertainty-aware prediction of 195Pt chemical shifts from limited data
CAI - D2 - O11	15:00-15:15	Muhammad Umer	Machine learning force fields for accelerated design and discovery of electrocathodic materials
CAI - D2 - O12	15:15-15-30	Paul Popelier	FFLUX: Machine Learnt Potentials based on Quantum Topological Atoms
CAI - D2 - O13	15:30-15:45	Sergey Varnavskiy	Data-centric AI in computational chemistry: integrating curated literature with other data
CAI - D2 - O14	15:45-16:00	Trung Trinh	Data-Driven Process Intensification of Methyl Acetate Production via Surrogate-Based Bayesian Optimization
Coffee break			

CAI - D2 - O15	16:30-16:45	Elham Sattarinezhad	Exploring the Mechanism of Protochlorophyllide to Chlorophyllide Conversion
CAI - D2 - O16	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
CAI - D2 - O17	17:00-17:15	Hilal Kalkan	Computational Screening of Triphenylamine-Based Star-Shaped Molecules: Insights into Electronic and Optical Properties for Organic Photovoltaic
CAI - D2 - O18	17:15-17:30	Steven Beutick	Lone-Pair Shielded Radicals: Beyond the Captodative Substitution Pattern
CAI - D2 - O19	17:30-17:45	Giovanni Bistoni	Novel computational strategies for the study of chemical selectivity: Combining high accuracy and chemical insight
CAI - D2 - O20	17:45-18:00	Christoph Plett	ORCA Meets Python – The ORCA Python Interface OPI

Posters			
CAI - D2 - P01		Sheu Sheh-Yi	Molecular quantum computer
CAI - D2 - P02		Verheyen Seppe	Towards circular design of thermoset polyurethanes: harnessing molecular dynamics and density functional theory for the depolymerization reactivity
CAI - D2 - P03		Jiang Yifan	Complex absorbing potentials for density functional theory
CAI - D2 - P04		Andrae Dirk	Accurate property data for small molecules from theory
CAI - D2 - P05		Nguyen Ha Quyen	Density functional methods for the theoretical modeling of Auger decay
CAI - D2 - P06		Wittemann Tobias	Dissociative electron attachment to building blocks of DNA studied by ab-initio molecular dynamics with complex absorbing potentials
CAI - D2 - P07		Sulkova Katarina	FNDMC as a tool for quantifying static and dynamic electron correlation in complex systems
CAI - D2 - P08		Oyo-Ita Inyang	Probing the impact of small molecules (X = N, P, S, Si) doped Covalent organic framework (X-COF) as sensors for ciprofloxacin pollutant
CAI - D2 - P09		Edet Henry	Heteroatoms (B, N, and P) doped on nickel-doped graphene for Phosgene ($COCl_2$) adsorption: insight from theoretical calculations
CAI - D2 - P10		Adriano Silva	Weak Global Correlations, Hidden Local Trends: Regime-Aware Analysis of Biochar Synthesis–Property Data

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

Session	Timing	Presenter	Title
CAI - D3 - O1	10:00-10:15	Simen Camps	Resolving spin contamination in spin-flip methods: the extended spin-flip CC2 method
CAI - D3 - O2	10:15-10:30	Hans Lischka	Machine learning and multireference configuration interaction for high-level nonadiabatic dynamics simulation of hexatriene
CAI - D3 - O3	10:30-10:45	Tommaso Giovannini	Driving Chemistry through Plasmonic Photoinduced Phenomena: An Atomistic Perspective
CAI - D3 - O4	10:45-11:00	Federico Rossi	Convex Hartree-Fock and Density Functional Theory for Stable Simulations at Conical Intersections
CAI - D3 - O5	11:00-11:15	Federica Borzelli	Computational modeling of tryptophan fluorescence spectra in proteins
CAI - D3 - O6	11:15-11:30	Francesco Di Maiolo	Organic Diradicals Bridged by Inverted Singlet-Triplet Units for Optical-Spin Interfaces
CAI - D3 - O7	11:30-11:45	Jordi Cirera	Data-Driven Prediction of Spin-Crossover Properties from Electronic Structure Calculations
CAI - D3 - O8	11:45-12:00	Jasper Schuurmans	Digital twins to design reactors for efficient photochemistry
POSTER FLASH	12:00		
CAI - D3 - F01		Tanimu Gazali	Ensemble Model Technique for Predicting the Yield of Dehydrogenation Products during the Oxidative Dehydrogenation of n-butane
CAI - D3 - F02		Cafiero Mauricio	Automated design of peptide-based scavengers using MLIPs and Boltz2
CAI - D3 - F03		Ivkovic Zarko	Data-driven reactivity design through generative modeling with quantum chemistry validation
CAI - D3 - F04		Laux Anika	Comparative Modelling of Biological Methanation Reactors for Sustainable CO_2 Conversion
CAI - D3 - F05			
CAI - D3 - F06		Zhang Chenfeng	Molecular Dynamics Insights into Ion Conduction and Gating Mechanisms of PKD2
CAI - D3 - F07		Sharma Manoj	Quantum Computational, Spectroscopic, Topological, Molecular Docking, and Dynamics Studies of 2-Amino-3-Hydroxypyridine (2A3HP): A Potential Antimicrobial Agent
Lunch			
CAI - D4- I1	14:00-14:30	**Rigoberto Hernandez**	
CAI - D3 - O9	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
CAI - D3 - O10	14:45-15:00	Hsin-Yi Tiffany Chen	Multiscale modeling of hydrogen coverage on Ru nanoparticle: a combined DFT, AIMD, and DPMD study
CAI - D3 - O11	15:00-15:15	Edoardo Panzetta	Computational study of N-methylacetamide (NMA) amide bond cleavage reaction in neutral and alkaline conditions
CAI - D3 - O12	15:15-15-30	Giulia Ciattaglia	A computational study of beta cyclodextrin-based nanosponge inclusion complexes
CAI - D3 - O13	15:30-15:45	Torsten John	From Mechanisms to Function: Computational Studies of Peptide Self-Assembly at Interfaces
CAI - D3 - O14	15:45-16:00	Horacio Poblete	Programmable Peptide–Graphite Interfaces for Water Bioremediation: From Gly–X Sequence to Ion Capture

CAI - D3 - O15	16:30-16:45	Silvia Casassa	CRYSTAL, an ongoing project for a theoretical chemical approach to solids
CAI - D3 - O16	16:45-17:00	Marta Corno	Multiscale approaches to drug encapsulation and release in β-cyclodextrin-based systems
CAI - D3 - O17	17:00-17:15	Bónis Barcza	Including charge transfer states in fragment based exciton calculations
CAI - D3 - O18	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
CAI - D3 - O19	17:30-17:45	Thomas Jagau	Recent progress in computational Auger spectroscopy
CAI - D3 - O20	17:45-18:00	Alistair Sterling	Seamless integration of machine-learned interatomic potentials into quantum chemistry workflows with ChemRefine

Coffee break

Posters

CAI - D3- P01	Shaikh Mohd Aatif	Design and synthesis and computational studies of 2-amino5,4b Thaizolopyrdine egfr based anti-cancer agent
CAI - D3- P02	Yuan Shaoxuan	From manual operation to autonomous STM via visual reasoning AI
CAI - D3- P03	Hussain Abrar	Novel Antimicrobial Agents: From Synthetic Design to Integrated In Vitro and In Silico Insights
CAI - D3- P04	Usman Jamilu	Data-Driven Process Optimization for Selective Magnesium Recovery from Desalination Brine
CAI - D3- P05	Millan Judith	Unravelling Aspartame Induced Activation Pathways in the TAS1R2/TAS1R3 Receptor
CAI - D3- P06	Calcagno Francesco	Quantum Computers For Molecular Inverse Design: The Quantum Ensemble Variational Optimization Algorithm
CAI - D3- P07	Levison Anna	The Role of Metal-Ligand Binding on Natural Product Inhibitors of Methyl-Coenzyme M Reductase
CAI - D3- P08	Silva Adriano	Automated Classification and Quantification of Pickering Emulsion Droplets Using YOLOv7
CAI - D3- P09	Zaid Mohd	A reproducible multi-scale computational workflow for DL-methionine in breast cancer targets: DFT, data-driven docking, MD and MM-PBSA validation
CAI - D3- P10	Maria Jaworska	Mechanism of methylation of A-cluster in coenzyme A synthase by cobalamin. Insight from DFT calculations

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

Session	Timing	Presenter	Title
CAI - D4 - O1	10:00-10:15	Rosie Gibson	The Evolution of AI in Scientific Searching
CAI - D4 - O2	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
CAI - D4 - O3	10:30-10:45	Jorge J. Carbó	3D-QTAIM Descriptor-Based Modeling for Asymmetric Catalysis
CAI - D4 - O4	10:45-11:00	Cheng-Chung Wang	AI and statistical analysis for understanding stereoselective glycosylation reactions
CAI - D4 - O5	11:00-11:15	Laura Falivene	Chiral Deep Eutectic Solvents as Catalysts for Asymmetric Synthesis: A Machine Learning–Driven Molecular Dynamics Design Tool
CAI - D4 - O6	11:15-11:30	Tobe Vorsselmans	Water and CO Desorption from Amorphous Carbon Surfaces: A Computational and Experimental Study
CAI - D4 - O7	11:30-11:45	Yongsheng Huang	Multi-Scale Investigation Of Triboelectric Nanogenerator: An Expanded DFT Calculation Based on Machine Learning
CAI - D4 - O8	11:45-12:00	Joep Wals	Binding mechanism of UAMC-1110 to Fibroblast Activation Protein
POSTER FLASH	12:00		
CAI - D4 - F01		Weiser Jonas	Towards automated ensemble-averaged kinetics of reverse intersystem crossing in flexible TADF emitters
CAI - D4 - F02		Sacchetta Filippo	Rhodopsin charge diffusion computations disclose contrasting color-tuning mechanisms
CAI - D4 - F03		Shekiladze Ilona	From Nature's Layers to Neural Layers: An AI and Machine Learning Approach to Tomato Preservation via an Edible Pseudoprotein Coating
CAI - D4 - F04			
CAI - D4 - F05		Kuchenbecker Vinicius	Theoretical study of collision induced dissociation mechanism for PO3G 77-59 m/z ion: When MS2 Energy Data and Quantum Chemistry reveals hidden molecular structures
CAI - D4 - F06		Karen Dsouza	Predictive Modeling of Ligand-Driven Lanthanide Separation for Critical Metal Separation Processing
CAI - D4 - F07			
Lunch			
CAI - D4 - I1	14:00-14:30	**Francoise Remacle**	Tentative title: Control of molecular reactivity with attopulses
CAI - D4 - O8	14:30-14:45	Marilù Maraldi	Realistic simulations of nonlinear optical photoswitches with novel all-atom quantum mechanical methodologies
CAI - D4 - O9	14:45-15:00	Markus Weiss	Asymmetrically-constrained Adiabatic ALMO-EDA: Designing Catalysts from First Principles
CAI - D4 - O10	15:00-15:15	Florian Matz	All correlation within a mean field: Assessment of i-DMFT and the modified Collins conjecture
CAI - D4 - O11	15:15-15:30	Abiche Ekalu	The roles of artificial intelligence in medicinal plants and natural products chemistry

Posters		
CAI - D4- P01	Shafique Aamir	Computational anharmonic thermoelectric transport in barium chalcogenide perovskites
CAI - D4- P02	Žagar Leon	Model Order Reduction of CFD Model for Membrane Distillation
CAI - D4- P03	Simon Nicolas	Plasma-Treated Poly(Lactic Acid): Deciphering the Structure of a Versatile Engineering Material
CAI - D4- P04	Yaşar Nesrin Işıl	Cross-validated screening of natural products targeting two distinct functional sites of the bacterial ribosome: An in-silico study
CAI - D4- P05	Roman Ventura Viviana	(η5-B5H10)Fe(η5-B5H10): A Novel Sandwich Complex analogue to Ferrocene
CAI - D4- P06	Francisca Salas	Beyond Bulk Aggregation: Interfacial Chloride Recognition by Triazolophane on Graphene
CAI - D4- P07	Carl Schiebroek	Balancing Data Quantity and Quality: Evaluating Curation Strategies for Bioactivity Prediction
CAI - D4- P08	Shanti Patra	Rationalizing the DCD model in transition metal carbonyls: a conceptual density functional theory analysis
CAI - D4- P09	Angel Rodriguez Leon	Assessing foundation variable-charge MLIPs for MoS2–ionic liquid interfaces: From benchmarks to fine-tuning
CAI - D4- P10	Umair Khan	Unified data-driven flow regime identification in horizontal and vertical multiphase pipe flows using dynamic pressure signals