

Monday 27th April – Session I

9:00–9:15	Opening	Noelia Romero López (National COST Coordinator) & Marta I. Hernández (Director of IFF-CSIC)	María Pilar de Lara-Castells (COST Action Chair) & Berta Fernández (Session Chair)
9:15–9:45	Overview I	Alessandro Fortunelli (CNR, Italy)	The COSY Working Group 3: “Confined Metal and Metal-Oxide Nanoparticles and Clusters Down to the Subnanometer Scale”
9:45–10:10	Invited Lecture	Stefan Vajda (Czech Academy of Science, Czech Republic)	From Single Atoms to Bimetallic Clusters and Nanostructured Surfaces: Selective Dehydrogenation & Hydrogen Production
10:10–10:35	Invited Lecture	María J. López (University of Valladolid, Spain)	Novel single-atom and single-cluster metal catalysts supported on carbon based layered materials
10:35–10:50	Contributed Talk	Lala Gahramanli (Baku State University, Azerbaijan)	Plasmonic–Semiconductor–Metal Oxide Synergy in a 2D/1D Graphene/Ag–Ag₂S–Ag₂O Photocatalyst for photocatalysis
10:50–11:05	Contributed Talk	Konstantin Neyman (ICREA & University of Barcelona, Spain)	When Platinum Becomes Not Noble: Platinum-Oxide Clusters Supported on Ceria
11:05–11:45	Coffee Break	“Claustro” Serrano 123	

Monday 27th April – Session II. Session Chair: Stefan Vajda (Czech Academy of Science, Czech Republic)

11:45–12:15	Overview II	Avelino Corma (UPV-CSIC, Spain)	Molecular Sieves for Reactions in Confined Spaces that Mimic Enzymatic Catalysts
12:15–12:40	Invited Lecture	Félix G. Requejo (UNLP and CONICET, Argentina)	Understanding Catalytic Clusters under Operando Conditions by XANES
12:40–13:05	Invited Lecture	Marinella Striccoli (CNR, Italy)	Controlled assembly of luminescent colloidal nanocrystals into highly ordered 3D superstructures
13:05–13:20	Contributed Talk	José R. B. Gomes (University of Aveiro, Portugal)	Breaking the Oxygen Shield for Reactivity Control in Mo₂C-Based MXenes
13:20–15:00	Lunch		

Monday 27th April – Session III. Session Chair: Heribert Reis (National Hellenic Research Foundation, Greece)

15:00–15:30	Overview III	Sonja Grubisic (University of Belgrade, Serbia)	Molecular Motion in Confined Systems: Advances in Simulations, Methods, and Models – WG2 Highlights
15:30–15:55	Invited Lecture	Kaido Sillar (University of Tartu, Estonia)	Chemically Accurate Ab Initio Prediction of Adsorption Thermodynamics and Isotherms in Metal–Organic Frameworks
15:55–16:20	Invited Lecture	Sergiy Perepelytsya (National Academy of Science, Ukraine)	Metallized Ag-DNA: Computational insights into a novel biomolecular material
16:20–16:35	Contributed Talk	Mikolaj Lewandowski (University in Poznań, Poland)	Iron nitrides under oxidizing conditions: What we know from model studies on 2D Fe(x)N islands on copper?
16:35–16:50	Contributed Talk	Avni Berisha (University of Prishtina, Kosovo)	How Oxide Nanocages Trap the Most Inert Greenhouse Gases
16:50–17:30	Coffee Break	“Claustro” Serrano 123	

Monday 27th April – Session IV. Session Chair: Alexandre Zanchet (IFF-CSIC)

17:30–17:55	Invited Lecture	Jorge M. C. Marques (University of Coimbra, Portugal)	Bio-inspired functionalization of chitosan for water remediation: computational insights into neonicotinoid sequestration
17:55–18:20	Invited Lecture	Teodora Kirova (University of Latvia, Latvia)	Theoretical study of the sensing properties of KL 1421 luminophore interacting with carotenoids

	Contributed Talk	Ateeque Malani (IIT Bombay, India)	Thermodynamics of confined water in swelling of clays
18:20–18:35	Contributed Talk	Jorge Alonso de la Fuente (IFF-CSIC, Spain)	Photoionization of phosphorous hydrides: experimental and theoretical comparison
Tuesday 28th April – Session V. Session Chair: Maria Krikunova (ELI Beamlines Facility, Czechia)			
9:00–9:30	Overview IV	Marcel Mudrich (University of Kassel, Germany)	Tracking microhydration of salt molecules by Penning ionization electron spectroscopy in helium nanodroplets
9:30–9:55	Invited Lecture	Kestudis Aidas (Vilnius University, Lithuania)	Structural and NMR properties of ionic liquid materials: insights from MD/QM modelling
	Invited Lecture	Francesca Mocci (Universita Degli Studi Di Cagliari, Italy)	Environmental Control of G-Quadruplex Stability: A Molecular Dynamics Perspective
9:55–10:10	Contributed Talk	David Lauvergnat (CNRS and Université Paris-Saclay, France)	Quantum Dynamics with a Smolyak scheme. Applications to clathrate hydrates
10:10–10:35	Contributed Talk	Nevin Uras-Aytemiz (Bandırma Onyedİ Eylöl University, Turkey)	First Principal Study of Defects in s-I and s-II Gas Hydrates
10:35–11:15	Coffee Break	“Calustro” Serrano 123	
Tuesday 28th April – Session VI. Session Chair: Alia Tadjer (University of Sofia “St. Kliment Ohridski”, Bulgaria)			
11:15–11:40	Invited Lecture	Paul Scheier (University of Innsbruck, Austria)	Experimental Solution of the Thomson Problem
11:40–12:05	Invited Lecture	Liudmil Antonov (Bulgarian Academy of Sciences, Bulgaria)	Make Tautomerism Great Again: New Challenges and New Possibilities
12:05–12:30	Invited Lecture	Massimiliano Bartolomei (IFF-CSIC, Spain)	Carbon Dioxide Preferential Adsorption and Conversion on Sodium Decorated γ-Graphyne
12:30–12:55	Contributed Talk	Nicolina Pop (Politechnica University of Timisoara, Romania)	Electron scattering on H_2^+, BeH^+ and their isotopologues: Dissociative recombination and ro-vibrational transitions
12:55–13:10	Contributed Talk	Milan Dimitrijević (Astronomical Observatory, Belgrade, Serbia)	Molecular data for characterization of confined molecular systems and corresponding databases
13:10–14:45	Lunch		
Tuesday 28th April – Session VII Session Chair: Aggelos Avramopoulos (University of Thessaly, Greece)			
14:45–15:10	Invited Lecture	Leticia González (University of Vienna, Austria)	Molecules in Confinement: How Environmental Shapes Reactivity and Photochemistry
15:10–15:35	Invited Lecture	Majdi Hochlaf (Gustave Eiffel University, France)	Spectroscopy and collisional dynamics of medium sized molecules
15:35–16:00	Invited Lecture	Dariusz Kędziera (Nicolaus Copernicus University in Torun, Poland)	Reliable PESs for Astrochemistry with autoPES: Methodology, Pitfalls, and Case Studies
16:00–16:15	Contributed Talk	Esther García-Arroyo (IFF-CSIC, Spain)	Selectivity of D_2/H_2 isotopologues by means of adsorption on a sodium-decorated graphene prototype: a quantum-mechanical low-pressure study
16:15–16:30	Contributed Talk	Andrew Cassidy (Aarhus University, Denmark)	Self-polarizing molecular films: confined electric fields in ices
16:30–17:00	Coffee Break	“Claustro” Serrano 123	
Tuesday 28th April – Session VIII. Session Chair: Marina Sekutor (Ruder Boskovic Institute, Croatia)			
17:00–17:25	Invited Lecture	Attila G. Csaszar (ELTE, Hungary)	Intriguing Manifestations of Noncovalent Interactions

17:25–17:50	Invited Lecture	Markus Meuwly (University of Basel, Switzerland)	Machine Learning Interactions for Chemical Reactions: Validation and Applications
17:50–18:15	Invited Lecture	Berta Fernández-Rodríguez (University of Santiago de Compostela, Spain)	Efficient Machine Learning barrier height and reaction enthalpy corrections for low- and mid-level quantum mechanical calculations
18:15–19:00	Flash Poster Presentations	Session Chair	Ljiljana Suručić (University of Banja Luka, Bosnia & Herzegovina)
Wednesday 29th April – Session IX. Session Chair: Henrik Grum Kjærgaard (University of Copenhagen, Denmark)			
9:00–9:30	Overview VII	Cristina Puzzarini (University of Bologna, Italy)	Modeling Reactivity under Interstellar Conditions
9:30–9:55	Invited Lecture	María Luisa Senent-Díez (IEM-CSIC, Spain)	Ab initio calculations applied to the study of organic non-rigid molecules with (at least) three interacting torsional modes.
9:55–10:20	Invited Lecture	Malgorzata Biczysko (University of Wrocław, Poland)	QM- and AI-based Approaches to the Structure and Spectroscopy of Biological Macromolecules
10:20–10:35	Contributed Talk	Magdalena Saldyka (University of Wrocław, Poland)	Photo-transformations of thiazole carboxylic acids in low temperature matrices
10:35–10:45	Contributed Talk	Justyna Krupa (University of Wrocław, Poland)	Matrix-Isolation Photochemistry: Experimental-Theoretical Insights for Astrochemical Complexity
10:45–11:00	Contributed Talk	Alessandra Savarese (University of Bologna, Italy)	Energetic and Spectroscopic Insights into the C₃H₆O₂ Isomer Family for Astrochemical Purposes
11:00–11:30	Coffee Break	“Claustro” Serrano 123	
Wednesday 29th April – Session X. Session Chair: Alberto García Vela (IFF-CSIC)			
11:30–11:55	Invited Lecture	Fernando Martín (Universidad Autónoma de Madrid, Spain)	New directions in Attosecond Chemistry
11:55–12:20	Invited Lecture	Ignacio Solá (Universidad Complutense de Madrid, Spain)	Steering Complex Photodissociation Dynamics through Initial Vibrational Coherences
12:20–12:45	Invited Lecture	Martin Quack (ETH Zurich, Switzerland)	High resolution spectroscopy, parity violation and quantum tunneling dynamics in chiral molecules of astrophysical and general interest
12:45–13:10	Invited Lecture	Vladimir Sreckovic (Institute of Physics Belgrade, Serbia)	Modeling Astrochemical Reaction Rates in Confined Molecular Environments
13:10–13:25	Contributed Talk	Stefan Bromley (University of Barcelona, Spain)	Identifying Observable Infrared Signatures of Nanosilicate Dust Grains in the Interstellar Medium
13:25–13:40	Contributed Talk	Manuel Mendoza-Hurtado (University of Córdoba, Spain)	Dual-locality learning under neighbourhood coupling: interpretable and transferable models for structured trace data
13:40–13:55	Contributed Talk	Abdulkadir Sezai Sarac (Istanbul Technical University, Turkey)	Confined Magnetic Ferrite Nanoparticles in Polyacrylonitrile Nanofibers: Tunable Nanostructures for Tissue Engineering
13:55–14:55	Lunch		
14:55-15:20	Best Contributed Talk and Poster Awards	Katarzyna M. Krupka (IFF-CSIC) & Manuel Mendoza Hurtado (University of Cordoba). Poster Awards, SPONSOR: RSC PCCP	María J. López (University of Valladolid) & Alessandro Fortunelli (CNR, Italy). Contributed Talk Awards, SPONSOR: Wiley Small Structures
15:20–15:50	Coffee Break	“Claustro” Serrano 123	
15:50–19:15	MC Meeting		
19:30–21:00	Get-together Event	“Claustro” Serrano 123	