Monday, 29.08.

08:00 Registration

Chair: David M. Smith

09:00 **Plenary Lecture II: Tim Clark**, Local Properties in Simulations of Charge Transport

09:45 **Christian R. Wick**, Semiempirical MO-Theory for Large Systems

10:10 **Chiara Panosetti**, Better (Random) Walking Through Chemistry: How Not to Get Lost in Vast Configurational Spaces

10:35 Break

11:00 **Janez Mavri**, How are Biogenic Amines Decomposed by Monoamine Oxidases: Lessons from Multiscale Simulation

11:35 **Jernej Stare**, Reaction Pathway Sampling by Empirical Valence Bond Simulation: From Gas Phase to Enzymes

12:00 **Danijela Barić**, Reduction of Ribonucleotide in Prebiotic Conditions

12:30 Lunch

12:50 DS: Tissues / Free Time

Chair: Borislav Kovačević

15:20 **Plenary Lecture III: Stefano Stranges**, Perspectives in Studying Free Radical-Surface Interaction by Synchrotron Radiation

16:05 **Ines Despotović**, Pyridine-Based Macrocyclic Compounds as an Efficient Tool for the Metal Cation Binding

16:30 Break

Chair: Zoran Miličević

17:00 **Sonia Coriani**, The Molecular Response to Electromagnetic Fields: A Wonderful Playground for a Computational Chemist

17:35 **Luca Grisanti**, Structure-Related Fluorescence and Proton Delocalization in Amyloid Proteins

18:00 **Marco Ruberti**, Coherence and Ionic State Produced After Multiphoton Molecular Ionization

18:25 **Antonio Prlj**, Challenges in Description of Optical and Electronic Properties of Heteroaromatic Molecules

18:45 Dinner

Chair: Aurora Ponzi

20:15 **Plenary Lecture IV: Maria Novella Piancastelli**, Acetylacetone Femtochemistry at FERMI-LDM

21:00 Refreshments at the Posters

Tuesday, 30. 08.

Chair: Damir Kralj

09:00 **Plenary Lecture V: Giuseppe Falini**, Biomaterials Inspired from Biomineralization

09:45 **Zlatko Brkljača**, Biomineralization and Biomineralization-Inspired Drug Design: Calcite-Peptide Interactions

10:10 **Lara Štajner**, Interaction between Calcium Carbonate and Selected Amino Acids

10:35 **Robert Stepić**, Theoretical Study of Amino Acid-Calcite Interface

10:55 Break

11:30 **Davor Kovačević**, Polyelectrolyte Multilayers: Properties and Applications

12:05 **Ali Hassanali**, Holes in Liquid Water and Other Hydrophobic Effects

12:40 **Zoran Miličević**, Effect of Electric Fields on Transport Properties of Small Solutes in Aqueous Environments

13:05 Lunch

13:40 DS: Calcite/Free Time

Chair: Zlatko Brkljača

16:30 **Marco Haumann**, Surface Influences on Catalytic Performance of Supported Ionic Liquid Phase (SILP) Materials

17:10 **Yaroslava Lykach**, Model Catalysis with Ionic Liquids

17:35 **Daniel Berger**, Multiscale Simulation of SILP Catalysis

18:00 **Christof Jäger**, Towards Engineering Radical SAM Enzymes – Insights into Biocatalysis and Biomaterial-Ionic Liquid interactions

18:25 **Nataša Vučemilović-Alagić**, Ionic Liquids at Interfaces

18:45 Dinner

Chair: Ana-Sunčana Smith

20:15 **Plenary Lecture VI: Jens Harting**, Soft Particles at Fluid Interfaces: the Interplay of Deformability and Surface Tension

21:00 Refreshments at the posters

Wednesday, 31.08.

Chair: Adriana Lepur

09:00 **Anđela Šarić**, Physical Determinants of Pathological Protein Aggregation

09:35 **Maryam Aliee**, Interaction of Polarity Fields Driving Pattern Formation in Tissues

10:00 **Robert Blackwell**, A Biophysical Model for the Formation of Mitotic Spindle Bipolarity

10:25 **Sara Kaliman**, Formation of Epithelial Tissues on Inorganic Functional Surfaces: Space Tessellation on Micro and Macro Scale

10:45 **David M. Smith**, Closing Remarks

11:00 DS: Ionic Liquids / Free Time

12:30 Lunch

Sunday, 28.08.

11:00	DS: Membranes
13:00	Lunch
14:00	Registration
15:00	**David M. Smith**, Opening Remarks

Chair: Ana-Sunčana Smith

15:10	**Plenary Lecture I: Sabine Maier,** On-Surface Synthesis and Self-Assembly of Molecular Nanostructures: From Metal to Insulator Surfaces
15:55	**Tajana Preočanin**, Charging of Solid Surface / Aqueous Interface: Surface Potential Measurements
16:30	Break

Chair: Nađa Došlić

17:00	**Milena Petković**, Formation and Oxidation of a P-$C_{carbone}$ Bond
17:35	**Aurora Ponzi**, TRPES as a Probe for Ultrafast Excited State Dynamics: an Exploratory Investigation of Furan
18:00	**Jurica Novak**, Photodynamics of Retinal Chromophore-Counterion Pairs
18:25	**Marin Sapunar**, Nonadiabatic Dynamics and Photoelectron Spectroscopy Simulations of Pyrrole
18:45	Dinner
20:15	Poster Session

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What?

The key project goal is to establish a network of professional training of young scientists in interdisciplinary research of innovative surfaces and materials.

Who?

The realization of the network will be under the supervision of a high-quality team of eminent scientists with complementary expertise, designed to simultaneously solve several related problems, all of which are of direct relevance to the project goals.

Why?

Response to problems in the research, development and innovation system: continuous brain drain of researcher personnel; lack of career supporting opportunities for junior and young researchers and a weak linkage between the science, research and business sector.

Workshop organizing committee:

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MIPOMat

Workshop Innovative Surfaces and Materials

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Primošten, Croatia

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Ruđer Bošković Institute

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