

## Sunday, 28.08.

10:00-	Registration	
11:00	Discussion Session* I: Membranes	
12:00-	Lunch	
15:00	Opening Remarks	Chair: Ana-Sunčana Smith
15:10	Plenary Lecture I: Sabine Maier <i>On-Surface Synthesis and Self-Assembly of Molecular Nanostructures: From Metal to Insulator Surfaces</i>	
15:55	Tajana Preočanin <i>Charging of Solid Surface / Aqueous Interface: Surface Potential Measurements</i>	
16:30	Break	Chair: Nađa Došlić
17:00	Milena Petković <i>Formation and Oxidation of a P-C<sub>carbone</sub> Bond</i>	
17:35	Aurora Ponzi <i>TRPES as a Probe for Ultrafast Excited State Dynamics: An Exploratory Investigation of Furan</i>	
18:00	Jurica Novak <i>Photodynamics of Retinal Chromophore-Counterion Pairs</i>	
18:25	Marin Sapunar <i>Nonadiabatic Dynamics and Photoelectron Spectroscopy Simulations of Pyrrole</i>	
18:45	Dinner	
20:15	Poster Session	

## Monday, 29.08.

08:00	Registration	Chair: David M. Smith
09:00	Plenary Lecture II: Timothy Clark <i>Local Properties in Simulations of Charge Transport</i>	
09:45	Christian R. Wick <i>Semiempirical MO-Theory for Large Systems</i>	
10:10	Chiara Panosetti <i>Better (Random) Walking Through Chemistry: How Not to Get Lost in Vast Configurational Spaces</i>	
10:35	Break	
11:00	Janez Mavri <i>How are Biogenic Amines Decomposed by Monoamine Oxidases: Lessons from Multiscale Simulation</i>	
11:35	Jernej Stare <i>Reaction Pathway Sampling by Empirical Valence Bond Simulation: From Gas Phase to Enzymes</i>	
12:00	Danijela Barić <i>Reduction of Ribonucleotide in Prebiotic Conditions</i>	
12:25-	Lunch	
12:50	Discussion Session II: 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 Discussion Session III: 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 R. 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*
- 10:50 Closing Remarks
- 11:00 Discussion Session IV: Ionic Liquids / Free Time
- 12:30 Lunch

\*Discussion Sessions are meant only for participants involved in the highlighted topics, representing free time for other participants (whoever additionally wants to participate is welcomed).