Math/Chem/Comp 2025 – 36th MC² Conference

Inter University Centre Dubrovnik, 2 – 6 June 2025

PROGRAMME

MONDAY, JUNE 2	
09:30 – 10:00	**REGISTRATION**
10:00 – 10:30	**CONFERENCE OPENING (Hrvoj Vančik / Jerzy Cioslowski)**
CHAIR: Hrvoj Vančik	
10:30 – 11:15	**Miquel Solà:** *An Assessment of Potential Double 2D- And 3D-Aromaticity in Three Different Scenarios*
11:15 – 12:00	**Jerzy Cioslowski:** *Natural Densitals*
12:00 – 12:15	**COFFEE BREAK**
12:15 – 13:00	**Filip Prątnicki:** *Accuracies of the One-Electron and On-top Two-electron Densities Obtained with the Full Configuration-interaction Employing Commonly Used Basis Sets*
13:00 – 13:45	**Henryk A. Witek:** *Exact Separation of Angular Momentum in Wave Functions of Few-particle Systems*
14:00 – 16:00	**LUNCH BREAK**
CHAIR: Filip Prątnicki	
16:00 – 16:45	**Mihai V. Putz:** *Modeling the Chemical Transition State Within Logistic Quantum Transition Frequency Picture*
16:45 – 17:30	**Haci Mehmet Baskonus:** *On the Investigation of DNA Model by Using Analytical Methods in Soliton Theory*
17:30 – 18:15	**Dariusz Szczepanik:** *TBA*
16:45 – 17:30	**Ariel F. Perez Mellor:** *Unimolecular Dissociation Kinetics and Ion–molecule Complex Pathways of Protonated Cyclo-diglycine Revealed by Graph-theoretical Analysis of Reactive Trajectories*

TUESDAY, JUNE 3	
CHAIR: Miquel Solà	
09:30 – 10:15	**Hrvoj Vančik:** *How Reliable are Physical Models in Chemistry*
10:15 – 11:00	**Bartosz Trzaskowski:** *Tight-binding Approaches to Study Polyoxometalates as Artificial Enzymes*
11:00 – 11:15	**COFFEE BREAK**
11:15 – 12:00	**Nađa Došlić:** *Trajectory Surface Hopping for Simulating Photoinduced Molecular Dynamics*
12:00 – 12:45	**Valera Veryazov:** *Crystal and Electronic Structure of Th:CaF_2*
13:00 – 15:00	**LUNCH BREAK**
15:00 – 18:00	***Scientific discussions***

WEDNESDAY, JUNE 4	
CHAIR: Henryk A. Witek	
09:30 – 10:15	**Dragutin Svrtan:** *Geometry of Point Particles. Symbolic Computer Verification of the Atiyah's Conjecture for Five Points in the Euclidean Plane*
10:15 – 11:00	**Tomislav Došlić:** *A Model of Random Sequential Adsorption with Blockade Range on a Ladder Graph*
11:00 – 13:00	**IAMC meeting**
14:00 – ...	**CONFERENCE EXCURSION AND DINNER**

THURSDAY, JUNE 5	
CHAIR: Jerzy Cioslowski	
10:30 – 11:15	**Slavko Radenković:** *Calculation of Magnetically Induced Current Density Using a Semiempirical Approach*
11:15 – 12:00	**Elizabeth Hartung:** *The p-anionic Clar Structures of a Fullerene*
12:00 – 14:00	**LUNCH BREAK**
14:00 – 17:00	**WORKSHOP: Tomasz A. Wesolowski:** *Challenges in the Approach to Multi-level Simulations of Electronic Structure Based on Frozen-density Embedding Theory*

FRIDAY, JUNE 6	
10:00 – 11:00	**POSTER SESSION**
11:00 - 11:30	**CONFERENCE CLOSING (Hrvoj Vančik / Jerzy Cioslowski)**

POSTER SESSION	
P01	Stipe Mustać, Viktor Pilepić *Computational Study of Weak Force Contributions to RNA Tetraloop Stability and Structure*
P02	Ali Chahine, Jean-Marc Sotiropolous, Panagiotis Karamanis *Quantum Chemical Rational Design of Organic Thermoelectric Materials*
P03	Predrag Novak, Jelena Parlov Vuković, Tomislav Jednačak, Ana-Marija Jagatić Korenika, Ana Jeromel, Ivana Tomaz, Tomica Hrenar, Sandra Rončević, Ivan Nemet, Ines Primožić, Vilko Smrečki *NMR Spectroscopy and Statistical Analysis in Characterization of Complex Mixtures*
P04	Olivera Tadić & Group of Students *Does Chem Need Math?*
P05	Igor Djerdj *Visible-light-Activated CO2 Photoreduction Over Ceria-based High-entropy Oxide Catalysts*