Math/Chem/Comp 2024 – 35th MC² Conference

Inter University Centre Dubrovnik, 3 – 7 June 2024

PROGRAMME

MONDAY, JUNE 3	
8:00 – 9:00	**REGISTRATION**
9:00 – 9:20	**CONFERENCE OPENING (Hrvoj Vančik / Jerzy Cioslowski)**
CHAIR: Jerzy Cioslowski	
9:20 – 10:00	**Michael Melgaard:** *Density Functional Theory With Magnetic Fields: A Spectral Approximation Scheme*
10:00 – 10:30	**Andreas Savin:** *A Modified Expression for the Hamiltonian Expectation Value Exploiting the Short-Range Behavior of the Wave Function*
10:30 – 11:10	**Tomasz A. Wesolowski:** *The Failure of Gradient Expansion Approximation in Case of the Bi-Functional for Non-Additive Kinetic Potential*
11:10 – 11:30	**COFFEE BREAK**
11:30 – 12:00	**Stephen G. Dale:** *Variational Density Functional Theory Using the Jax Deep-Learning Differentiable Framework*
12:00 – 12:40	**Jacek Karwowski:** *Reflections on a Certain Density Functional: Is This a Warning or Maybe Ariadne's Thread?*
12:40 – 13:10	**Artur Ishkhanyan:** *Generalisation of the Second Demkov-Kunike Level-Crossing Quantum Two-State Model*
13:10 – 15:00	**LUNCH BREAK**
CHAIR: Andreas Savin	
15:00 – 15:30	**Katharina Boguslawski:** *Toward Alternative Wave Function Ansätze for Organic Electronics*
15:30 – 16:30	**John M. Herbert:** *High-Fidelity Fragmentation Methods in Quantum Chemistry*
16:30 – 16:50	**COFFEE BREAK**
16:50 – 17:30	**Miquel Solà:** *NICS and Ring Currents - An Exploration of Failures and Limitations*
17:30 – 18:00	**Valera Veryazov:** *Electronic Structure of Ionic Crystals with Ab Initio Methods*
18:00 – 18:40	**Branimir Bertoša:** *Allosteric Mechanisms of Selected Manganese Metallosensors*

TUESDAY, JUNE 4	
CHAIR: Henryk Witek	
9:00 – 10:00	**Jerzy Cioslowski:** *Symmetry Equiincidence of Natural Orbitals*
10:00 – 10:30	**Anjan Sadhukhan:** *Separation of Rotational Degrees of Freedom in Quantum Three-Body System*
10:30 – 11:30	**Hazel Cox:** *Bound State Stability in Few Particle Systems Using Numerical Methods*
11:30 – 12:00	**Jacek Komasa:** *Rovibrational Energy Levels of the Hydrogen Molecule and Its Isotopologues from Relativistic Nonadiabatic Calculations*
12:00 – 12:20	**COFFEE BREAK**
12:20 – 13:20	**Sergiy Bubin:** *Accurate Calculations of Few-Electron Systems Using Explicitly Correlated Wave Functions*
13:20 – 13:50	**Monika Stanke:** *Fine Structure of the Doublet P Levels of Five-electron Atomic Systems Calculated without the Born–Oppenheimer Approximation*
13:50 – 14:10	**Seiichiro L. Ten-no:** *Nonunitary Projective Transcorrelation Inspired by the F12 Ansatz*
14:10 – 16:00	**LUNCH BREAK**
CHAIR: Miquel Solà	
16:00 – 16:30	**Tetsuya Taketsugu:** *Dimensionality Reduction Techniques for Chemical Reactions: Reaction Space Projector and Natural Reaction Orbitals*
16:30 – 17:00	**Takao Tsuneda:** *Exploring the Connection Between Electronic and Potential Energy Theories via Reactive Orbital Energy Theory*
17:00 – 17:10	**COFFEE BREAK**
17:10 – 17:40	**Dirk Andrae:** *Many-to-One Mapping in Electronic Structure Calculations for Finite and Infinite Systems*
17:40 – 18:20	**Robert Berger:** *Discrete Symmetries in Systems of Indistinguishable Particles*
18:20 – 19:00	**Rahul Maitra:** *Error Mitigation Strategies for Near-Term Quantum Algorithms*

WEDNESDAY, JUNE 5	
9:00 – 12:00	**WORKSHOP** **Henryk A. Witek**: *Special Topics in the Theory of Angular Momentum*
14:30	**CONFERENCE TRIP**

THURSDAY, JUNE 6	
CHAIR: Henryk A. Witek	
9:00 – 11:00	**IAMC meeting**
11:00 - 11:20	**COFFEEBREAK**
11:20 – 11:50	**Douglas J. Klein:** *Orbital-Interaction Graphs for Saturated Hydrocarbons*
11:50 – 12:10	**Tomislav Došlić:** *Cluster Analysis of Fullerene Isomers*
12:10 – 12:30	**Ali Iranmansh:** *Exploring Degree-Based Graph Invariants in Random Graphs and Chains*
12:30 – 12:50	**Gašper Domen Romih:** *On I_1-embeddability of (Chemical) Hypergraphs*
12:50 – 14:30	**POSTER SESSION**
14:30 – 16:00	**LUNCH BREAK**
CHAIR: John M. Herbert	
16:00 – 16:20	**Bartosz Trzaskowski:** *Fast Computational Methods to Study Large and Complex Molecular Systems*
16:20 – 16:50	**Cristopher Camacho:** *A GPU-Accelerated Implementation of the Density-functional Tightbinding Method*
16:50 – 17:20	**Iulia Emilia Brumboiu:** *Core-Hole Delocalization Effects in Computational X-ray Spectroscopy*
17:20 – 18:00	**Sanja Tomić:** *Protein interactions of dipeptidyl peptidase III*

FRIDAY, JUNE 7	
9:00 – 10:00	**Urban Bren:** *Unravelling the Molecular Mechanism of Antimicrobial Activity of Tannins through Joint Experimental and Computational Means*
10:00 – 10:40	**Marcin Andrzejak:** *Coherent Vibrational Wave-packets in Singlet Fission – Theoretical Modeling of the Impulsive Vibrational Spectra*
10:40 – 11:00	**Nađa Došlić:** *Steering Excited State Proton Transfer: An Interplay of Electronic and Structural Factors*
11:00 - 11:20	**COFFEE BREAK**
11:20 – 11:50	**Azzam Alfarraj:** *Geometric Algebra Approaches to Protein-protein Docking*
11:50 – 12:20	**Paweł Tecmer:** *Reliable Description of Large Organic Molecules with PCCD-Based Methods*
12:20 – 12:50	**Bono Lučić:** *Improved Evaluation Metrics of Classification and Language Models in Chemistry and Beyond*
12:50 – 13:20	**Terry J. Frankcombe:** *The Hitchiker's Guide to the Wavefunction*
13:20 - 13:30	**CONFERENCE CLOSING (Hrvoj Vančik / Jerzy Cioslowski)**

POSTER SESSION	
P01	**Kammegne T. Brice, Michael Melgaard, and Hazel Cox:** *Using Numerical Tensor Methods for Solving the Many-Body Schrödinger Equation*
P02	**Tieu-Long Phan, Klaus Weinbauer, Peter F. Stadler:** *Reaction Rebalancing: A Novel Approach to Curating Reaction Databases*
P03	**Gabrijel Zubčić, Valerije Vrček, Viktor Pilepić, Davor Šakić and Erim Bešić:** *A Quantum Chemical Insight into Radical Rearrangements in the Single Crystal of 2-Thiothymine*
P04	**Olivera Tadić & group of students:** *Do Biometric Measurements of Trees Need Mathematics?*
P05	**Igor Djerdj, Stjepan Šarić, Dalibor Tatar, Jelena Kojčinović, Ronen Gottesman, Oded Millo, Doron Azulay, Habib Ullah:** *Rare-Earth High-Entropy Oxides – Driven Enhancement of Ceria's Photocatalytic Watter Splitting: Experiment and DFT Study*
P06	**Erika M. Herrera Machado, Jakob L. Andersen, Rolf Fagerberg, Daniel Merkle:** *A Sensitivity Analysis of the Formose Chemistry with Borate Using Rule-Based Stochastic Simulations*
P07	**Kurt Varmuza, Matthias Dehmer, and Peter Filzmoser:** *Molecular Descriptors Based on Automorphism Data*
P08	**Deza Amistas, Christoph Flamm, and Peter Dittrich:** *Chemical Organisations in Stochastic Rare Event Simulations of Rule-Based Chemical Systems*