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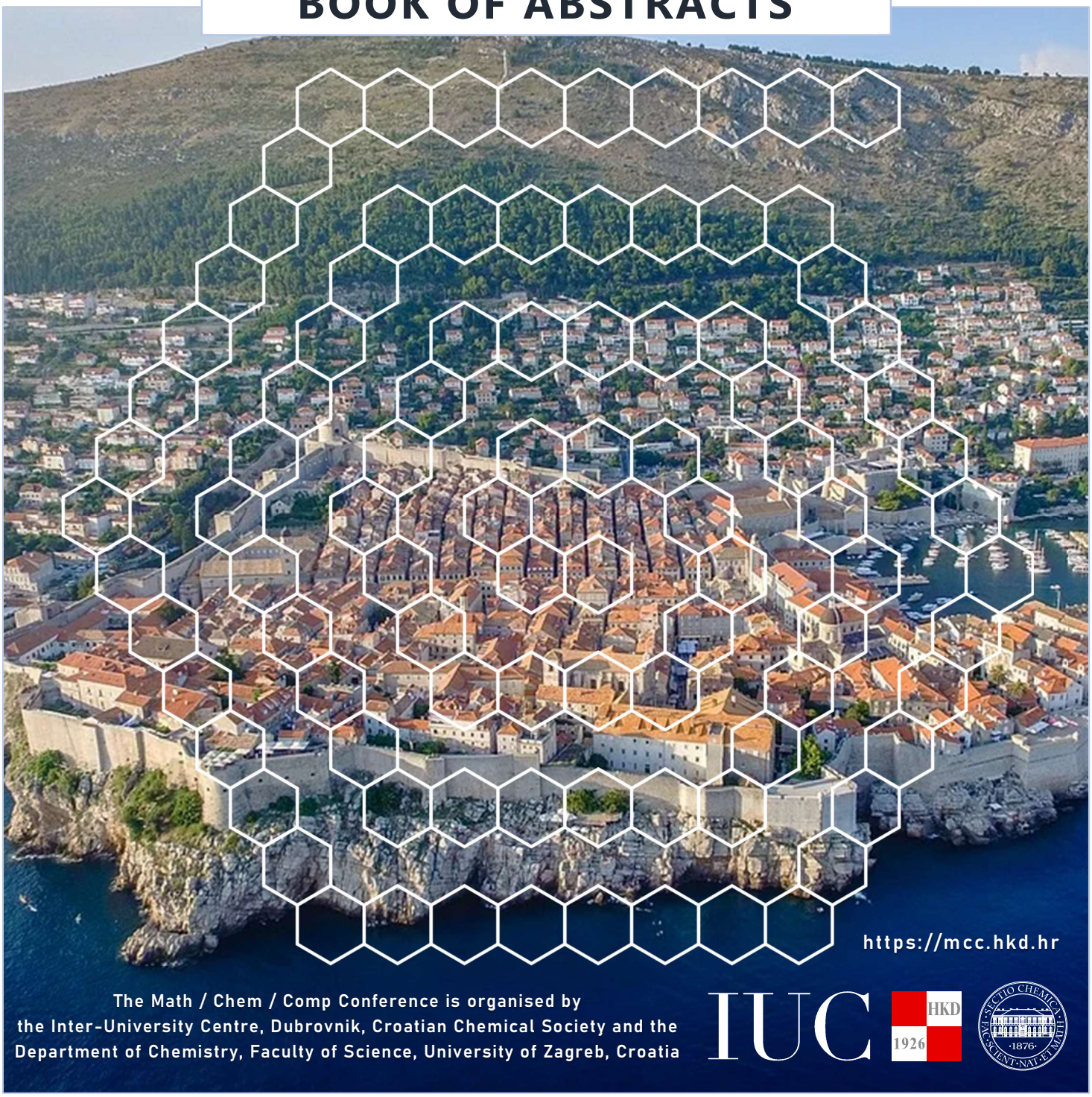
Math/Chem/Comp 2025 – 36th MC² Conference

Inter University Centre Dubrovnik, 2 – 6 June 2025

BOOK OF ABSTRACTS



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Department of Chemistry, Faculty of Science, University of Zagreb, Croatia

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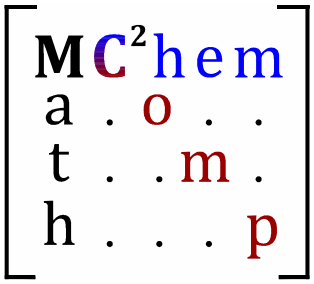

Math/Chem/Comp 2025 – 36th MC² Conference

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IMPRESSUM

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Zagreb, 2025

The 36th International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences: Mathematics, Chemistry, Computing (Math/Chem/Comp, MC^2-36)

Since 1986, the Math/Chem/Comp meetings have been bringing together researchers working on diverse subjects spanning mathematics, computer science, and chemistry. In continuation of this tradition, presentations concerning all aspects of current research on computer modeling, combinatorics, graph theory, and topology applied to any area of chemistry, physics, material and life sciences will be welcomed. The conference program will include invited plenary and special lectures workshops and posters. In particular, the MC^2-36 meeting will revolve around the following topics:

1. Mathematical methods and computational algorithms in modeling of atoms, molecules, and chemical processes
2. Mathematical chemistry and chemical graph theory
3. Molecular modeling in practice (including molecular dynamics and aggregation)
4. Chemical experiments, industrial processes, and mathematical interpretation

The conference program will include invited lectures, contributed oral presentations, and posters. Moreover, we will offer a **Workshop**: "Challenges in the frozen-density embedding theory based strategy for multi-level simulations of electronic structure" which will be held by Professor **Tomasz A. Wesolowski**, Department of Physical Chemistry, University of Geneva.

Proceedings

The papers presented at the MC^2-36 meeting can be submitted to *Croatica Chemica Acta* to be published as proceedings.

All contributions will be refereed. The participants are encouraged to submit their manuscripts before the meeting or at the latest upon arrival in Dubrovnik. Those unable to attend are invited to send their manuscripts to the director of the conference.

Hrvoj Vančik and Jerzy Cioslowski

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CONTENTS

LECTURES

Miquel Solà
An Assessment of Potential Double 2D- And 3D-Aromaticity in Three Different Scenarios..... 13

Jerzy Cioslowski
Natural Densitals..... 14

Filip Prątnicki
Accuracies of the One-Electron and On-top Two-electron Densities Obtained with the Full Configuration-interaction Employing Commonly Used Basis Sets..... 15

Henryk A. Witek
Exact Separation of Angular Momentum in Wave Functions of Few-particle Systems..... 16

Mihai V. Putz
Modeling the Chemical Transition State Within Logistic Quantum Transition Frequency Picture..... 17

Haci Mehmet Baskonus
On the Investigation of DNA Model by Using Analytical Methods in Soliton Theory 18

Dariusz Szczepanik
TBA 19

Ariel F. Perez Mellor
Unimolecular Dissociation Kinetics and Ion–molecule Complex Pathways of Protonated Cyclo-diglycine Revealed by Graph-theoretical Analysis of Reactive Trajectories..... 20

Hrvoj Vančik
How Reliable are Physical Models in Chemistry..... 21

Bartosz Trzaskowski
Tight-binding Approaches to Study Polyoxometalates as Artificial Enzymes 22

Nađa Došlić
Trajectory Surface Hopping for Simulating Photoinduced Molecular Dynamics..... 23

Valera Veryazov
Crystal and Electronic Structure of Th:CaF_2..... 24

Dragutin Svrtan
Geometry of Point Particles. Symbolic Computer Verification of the Atiyah's Conjecture for Five Points in the Euclidean Plane 25

Tomislav Došlić
A Model of Random Sequential Adsorption with Blockade Range on a Ladder Graph 26

Slavko Radenković
Calculation of Magnetically Induced Current Density Using a Semiempirical Approach..... 27

Elizabeth Hartung
The p-anionic Clar Structures of a Fullerene 28

WORKSHOP

Tomasz A. Wesolowski
Challenges in the Approach to Multi-level Simulations of Electronic Structure Based on Frozen-density Embedding Theory 31

POSTERS

Stipe Mustać, Viktor Pilepić
Computational Study of Weak Force Contributions to RNA Tetraloop Stability and Structure 35

Ali Chahine, Jean-Marc Sotiropolous, Panagiotis Karamanis
Quantum Chemical Rational Design of Organic Thermoelectric Materials 36

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 37

Olivera Tadić & Group of Students
Does Chem Need Math? 38

Igor Djerdj
Visible-light-Activated CO_2 Photoreduction Over Ceria-based High-entropy Oxide Catalysts 39

PARTICIPANTS

PARTICIPANTS 41

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*

LECTURES

AN ASSESSMENT OF POTENTIAL DOUBLE 2D- AND 3D-AROMATICITY IN THREE DIFFERENT SCENARIOS

Miquel Solà,[a] Sílvia Escayola,[a] Nathalie Proos Vedin,[b] Albert Poater,[a] Francesc Teixidor,[c] Clara Viñas,[c] Jordi Poater,[d] Slađana Đorđević[e], Slavko Radenković,[e] and Henrik Ottosson[b]

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The most widely known example of a species with double 2D-aromaticity is the hexaiodobenzene dication, $[C_6I_6]^{2+}$.[1] This species shows π-aromaticity in the benzene ring and σ-aromaticity in the outer ring formed by the iodine substituents. To our knowledge, no species with double 3D-aromaticity have been reported to date. Inspired by the hexaiodobenzene dication example, in this work, we explore the potential for double aromaticity in three different type of compounds: periodo-polycyclic aromatic hydrocarbons,[2] double 2D-aromaticity in tropylium (tri)cation and anion derivatives[3] and double 3D-aromaticity in $[B_{12}I_{12}]^{0/2+}$.[4] Our results based on electronic, magnetic, and energetic indicators of aromaticity show the presence of double aromaticity in several periodo-polycyclic aromatic hydrocarbon, in triplet $C_7Br_7^{+3}$ with an internal Hückel aromatic tropylium ring and an external incipient Baird aromatic Br_7 ring, but not in $[B_{12}I_{12}]^{0/2+}$.

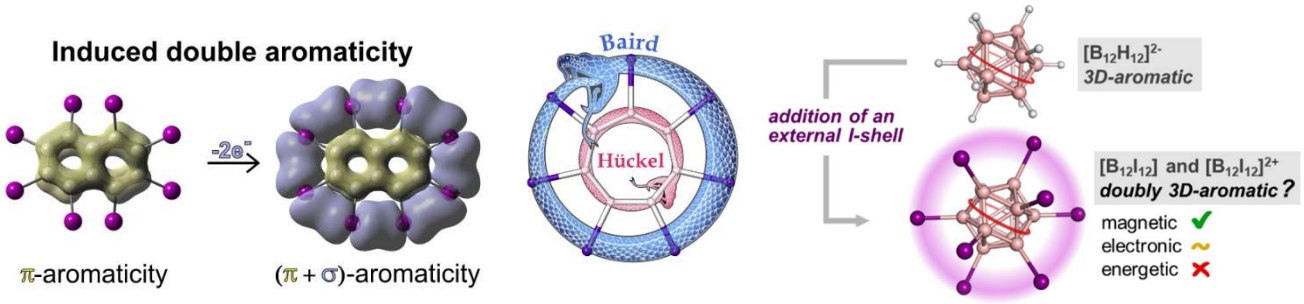

Figure 1. Some of the species described in this lecture

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NATURAL DENSITALS

Jerzy Cioslowski

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The concept of natural densitals (NDs) and their amplitudes is introduced. These quantities provide the spectral decomposition of the cumulant $D_2(\mathbf{x}_1, \mathbf{x}_2)$ of the two-electron density that, by definition, quantifies the extent of electron correlation. Consequently, they are ideally suited for a rigorous description of electron correlation effects in Coulombic systems. Spin-summed and spin-resolved versions of the NDs and their amplitudes are defined, and their properties are discussed in detail. Unlike the nonnegative-valued occupation numbers of the natural orbitals (NOs), these amplitudes exhibit diverse sign patterns that emerge within different regimes of electron correlation. The descriptive power of this property is vividly illustrated with the ground state of the H_2 molecule, in which the subtle interplay of various types of electron correlation is captured in detail by a straightforward examination of the amplitudes of the NDs alone. Offering the most compact bilinear representations of $D_2(\mathbf{x}_1, \mathbf{x}_2)$ (a property analogous to that of the NOs with respect to the 1-matrix), the NDs open entirely new vistas in the analysis of electronic structures of atoms and molecules.

ACCURACIES OF THE ONE-ELECTRON AND ON-TOP TWO-ELECTRON DENSITIES OBTAINED WITH THE FULL CONFIGURATION-INTERACTION EMPLOYING COMMONLY USED BASIS SETS.

Filip Prątnicki

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In this talk, I will present accuracy studies of the one-electron density, the two-electron on-top density, and the on-top ratio, in which the ground-state wavefunction of the dihydrogen molecule was approximated by a linear combination of explicitly correlated Gaussian functions, and the results juxtaposed with these stemming from full Configuration Interaction (CI) method with commonly used correlation-consistent orbital basis sets. Since these quantities are employed in a broad spectrum of different formalisms and usually derived from wavefunction approximations typically assessed solely in terms of energy convergence, this research demonstrates that the energy error alone cannot serve as the sole criterion for establishing a foundation for reliable conclusions concerning even the simplest two-electron systems.

As the results reveals relative error amounting to ca. 1% may be achieved and maintained for one-electron density in full-CI calculations, while the accuracy of on-top two-electron density is affected by excessively high errors. Even with very large basis sets, these errors are not lowered to less than approximately 15%, but even that is possible only in close proximity to the nuclei. The obtained results also indicate that the on-top ratio values never exceed 1 for the considered systems, which was suggested in the literature. As these quantities are commonly employed in description and analysis of different types of electron correlation [1] or in DFT formalisms [2] some of the conclusions stated in such studies might be jeopardized. A brief illustration of such potentially unjustified conclusions arising from mentioned properties will be provided.

Acknowledgements. This work has been supported by the National Science Center (Poland) under grant 2022/47/B/ST4/00002. A significant portion of the results has been obtained using resources provided by Wroclaw Centre for Networking and Supercomputing (http://wcss.pl).

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EXACT SEPARATION OF ANGULAR MOMENTUM IN WAVE FUNCTIONS OF FEW-PARTICLE SYSTEMS

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Consider a quantum system (an atom or a small molecule) as a collection of N particles (electrons and nuclei), each of them carrying its own partial momentum and partial angular momentum. Since, the total momentum operator P and the total angular momentum operator L commute with the Hamiltonian H of the system, it is possible to identify three degrees of freedom for each of these operators and seperate them exactly in the wave functions corresponding to the system. While the separation of the degrees of freedom asociated with P is well-known (separation of the center of mass), the exact separation of the degrees of freedom associated with L is more complicated and consequently less-known.

The current paper is supposed to review the situation in the field and discuss in detail the family of minimal multipolar harmonics (see [1] for a thorough review of related topics) that can be used to derive reduced Schrödinger equation in 3N-6 variables for systems with well-defined quantum numbers corresponding the definite arbitrary values of the total momentum P, the total angular momentum L, and its projection M.

Acknowledgements. This work has been supported by the grant NSTC 113-2113-M-A49-001- funded by National Science and Technology Council of Taiwan.

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MODELING THE CHEMICAL TRANSITION STATE WITHIN LOGISTIC QUANTUM TRANSITION FREQUENCY PICTURE

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The fundamental thermdynamic entropy equation is employed to develop a quantum transition frequency picture considering the vibrational form for the Gibs energy of reaction (or reactivity) $-\Delta G = \hbar \upsilon_{mn}$. The result is that the formal solution for the quantum frequency within transition state for the given reaction aka transition triggering the reactivity is obtained for the first time in terms of W-Lambert function [1]; At this point the logistic equivalence for treating activated complex in the enzyme (enzyme-substrate ES) kinetics may also apply, $f_1 W\left(f_2 e^{f_2} e^{f_3}\right) \to f_1 \ln\left(1+\left(e^{f_2}-1\right)e^{f_3}\right)$ [2], yielding with the new insight in the quantum treatment of transition state, i.e. proofing the zero entropy and full quantum information transfer with the activated complex thereof. Further exploration of complex phenomena involving multiple channels in- and out- of transition states, e.g. for the photo-catalysis of water or hydrogen peroxide dissociation on TiO_2 (anatase) nano-surfaces, may provide new tools in analyzing, conducting and predicting molecular fragments and of their surface-path dynamics under specific nano-technical conditions [3].

Acknowledgements. This work has been supported by West University of Timisoara (DEVELOP Programme 2025) and by National Institute of RD for Electrochemistry and Condensed Matter (INCEMC "Nucleu" Programme 2025), respectively.

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ON THE INVESTIGATION OF DNA MODEL BY USING ANALYTICAL METHODS IN SOLITON THEORY

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In modern life, scientists have focused on the observations of the real world problems by using multidisiplinary properties. In such case, they aims to find the deeper properties of real reasons of problems. This type of multidisiplinary work render possible to better understand the nature of the real world problems arising in various fied of life. Therefore, in this study, we investigate the new and novel properties of DNA model [1,2] by using various analytical methods. From the results obtained in this study, it is estimated that these resuls may be a usefull tool to explain the deeper properties of te governeng model.

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TBA

UNIMOLECULAR DISSOCIATION KINETICS AND ION–MOLECULE COMPLEX PATHWAYS OF PROTONATED CYCLO-DIGLYCINE REVEALED BY GRAPH-THEORETICAL ANALYSIS OF REACTIVE TRAJECTORIES

Ariel F. Perez Mellor,[a] Thomas Burgi,[a] Riccardo Spezia[b]

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The talk introduces an automated workflow that converts ensembles of on-the-fly chemical-dynamics trajectories into a concise reaction network via permutation-invariant canonical labelling, depth-first fragmentation analysis, and centre-of-mass clustering[1,2]. Applied to the three protonated cyclo-diglycine isomers CYC^{00}, LIN^{00}, and OXA^{00}, the protocol resolves all primary fragmentation channels and their kinetics.

A minimal three-state scheme, parametrised with Rice–Ramsperger–Kassel (RRK) theory, directly yields microcanonical rate constants and energy thresholds from the ensemble data. OXA^{00} displays a distinct kinetic landscape: early formation of long-lived ion–molecule complexes restricts phase-space exploration, enabling roaming pathways that lower both the isomerisation barrier and the overall fragmentation threshold relative to the most stable isomer, CYC^{00}, in quantitative agreement with experimental CID spectra.

The workflow delivers picosecond rate constants without manual intervention by integrating graph theory, statistical kinetics, and high-throughput computation. It readily applies to mass-spectrometric fragmentation, photochemistry, and catalytic reaction analysis.

Acknowledgements. This work was partially supported by ANR DynBioReact (Grant No. ANR-14-CE06-0029-01) and the University of Geneva.

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HOW RELIABLE ARE PHYSICAL MODELS IN CHEMISTRY

Hrvoj Vančik

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Chemical concepts such as stability and reactivity are traditionally considered by using the standard physical methods: quantum mechanics (quantum chemistry) and thermodynamics. Here are discussed two case studies in which the deeper interaction between chemistry and physics is required for explanation of the investigated chemical phenomena, rather than an uncritical use of the *a priori* physical background.

The first example is the mechanistic interpretation of the polymerization kinetics of dinitrosoaromatic compounds in the solid state starting with the general physical approach to the study of solid-state processes.[1] The second case is the quantum chemical interpretation of the thermodynamics of the dimerization equilibrium of the simple aromatic nitroso compounds in solution.[2] From both the examples it follows, that the physical interpretation of chemical phenomena is not possible by using the basic physical approach exclusively. The rigorous interpretations of chemical behaviour require a fine-tuned two-directional interaction of chemical and physical concepts.

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TIGHT-BINDING APPROACHES TO STUDY POLYOXOMETALATES AS ARTIFICIAL ENZYMES

Bartosz Trzaskowski

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Polyoxometalas and other metal-oxo clusters are frequently found as building blocks in metal organic frameworks (MOFs) that are able to mimic the reactivity of biological enzymes and perform important catalytic reactions.[1] Due to their size and presence of transition metals, such systems are difficult to model using standard DFT methods or approaches based on classical force field models. To overcome these problems, we designed a new computational protocol combining molcular docking with the GFN2-xTB tight-bindind method to model these systems.

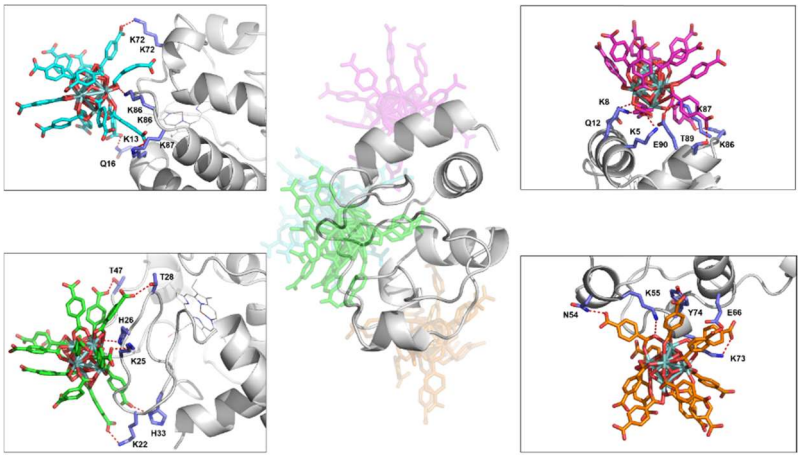

Figure 1. UiO-66 Zr node interacting with cytochrome.

We show that Zr-based artificial enzymes have peptidase activity and can accelerate peptide bond hydrolysis 10,000-fold with respect to the uncatalyzed reaction. Based on molecular modeling we show why Zr12-based MOF is initially faster than Zr6-based MOF, but yields an overall slower reaction by taking a longer time to afford the same reaction yield. the slower conversion is caused by the strong affinity of the Zr12 cluster for the product glycine.[2] We also show that this system is able to hydrolyze cytochrome and our computational approach allows to better understand the mechanism behind MOF-assisted protein hydrolysis.

Acknowledgements. This work has been supported by the Central Europe Leuven Strategic Alliance grant CELSA/24/007.

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TRAJECTORY SURFACE HOPPING FOR SIMULATING PHOTOINDUCED MOLECULAR DYNAMICS

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Nonadiabatic molecular dynamics methods are essential for the theoretical investigation of photochemical and photophysical processes triggered by light absorption. Among them, trajectory surface hopping (TSH) stands out for its balance between computational efficiency and physical interpretability. In this talk, I will present an overview of the TSH method and provide practical guidance for its accurate implementation. I will discuss key strategies for simulating nonadiabatic dynamics and demonstrate how TSH, when combined with accurate electronic structure calculations and appropriate analysis techniques, can reproduce experimental observables and uncover mechanistic insights into complex excited-state processes. I will show selected examples to highlight the strengths of the method and its usefulness for studying how molecules behave after absorbing light.[1,2]

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CRYSTAL AND ELECTRONIC STRUCTURE OF Th:CaF_2

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^{229}Th:CaF_2 is a promising material for use in atomic clocks. Despite intensive experimental and theoretical efforts, several aspects of this system remain unresolved. Even the crystal structure is under debate, due to the non-isovalent substitution of Ca^{2+} by Th^{4+} ions. Periodic calculations can only be performed at the density functional theory (DFT) level. These calculations suggest that Th substitution is stabilized by the presence of two additional fluorine ions near the Th site. However, the DFT-predicted electronic properties—such as the absorption spectrum and the electric field gradient—are inconsistent with experimental observations.

Using an embedded cluster model[1], we performed multiconfigurational calculations (CASSCF/CASPT2)[2] to explore the local crystal structure and electronic properties[3]. Because the precise structure near the Th site is unknown, we investigated several models: (i) direct Ca → Th substitution, (ii) substitution with an accompanying Ca vacancy, and (iii) substitution with two interstitial fluorine ions. Comparison of the calculated absorption spectra with experimental data allows us to rule out the model with two interstitial F^- ions. The electric field gradient, which can be directly measured via NMR and is highly sensitive to local structure, also supports our conclusions. Our results, in contrast to previous DFT predictions, agree well with experimental measurements. Although total energies from cluster calculations cannot directly determine the thermodynamic stability of the various defect structures, we performed a Born–Haber cycle analysis to estimate relative stabilities. This analysis also indicates that the structure involving two interstitial fluorine ions is less stable. Finally, analysis of the electronic structure[4] shows that electron distribution adapts to compensate the additional charge introduced by the Th^{4+} ion.

Acknowledgements. This work has been supported by NAWA grant BNI/PST/2023/1/00013/U/00001 and eSSENCE grant LU:11.2

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GEOMETRY OF POINT PARTICLES. SYMBOLIC COMPUTER VERIFICATION OF THE ATIYAH'S CONJECTURE FOR FIVE POINTS IN THE EUCLIDEAN PLANE

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In 2001 Sir M. F. Atiyah formulated a conjecture C1 and later with P. Sutcliffe two stronger conjectures C2 and C3. These conjectures, inspired by physics (spin-statistics theorem of quantum mechanics), are geometrically defined for any configuration of n points in the Euclidean three space. The conjecture C1 is proved for n = 3 in [1] and for n = 4 in [2], and C1' C3 in [3]. After two decades we succeeded in verifying C1 for arbitrary five points in the Euclidean plane. The computer symbolic certificate produces a new remarkable universal ('hundred pages long') positive polynomial invariant (for any five planar points), in terms of newly discovered shear coordinates. This refines the original Atiyah's conjecture and we are optimistic for its verification for n greater than five, (less optimistic ... 'It remains a conjecture for 300 years (like Fermat)' (see Atiyah: Edinburgh Lectures..2010). In the year 2013 Atiyah's conjectures were put on the new list of Nine open problems (from [4]) ('probably' easier than the remaining six out of famous Seven Clay millennium problems).

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A MODEL OF RANDOM SEQUENTIAL ADSORPTION WITH BLOCKADE RANGE ON A LADDER GRAPH

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In random sequential adsorption (RSA), objects are deposited on a substrate randomly, irreversibly, and sequentially. Attempts of deposition that lead to an overlap with previously deposited objects are discarded. The process continues until the system reaches a jammed state when no further additions are possible. We analyze a class of RSA models on a two-row square ladder graph in which landing on an empty site in a graph is allowed when at least b neighboring sites in the graph are unoccupied ($b \in \boldsymbol{N}$). In both dynamic and static settings we provide explicit expressions for key statistics that describe the average proportion of the substrate covered by deposited objects, and then we comment on significant differences between the two settings. We illustrate all of our findings through a toy model for ensembles of trapped Rydberg atoms with blockade range b.

CALCULATION OF MAGNETICALLY INDUCED CURRENT DENSITY USING A SEMIEMPIRICAL APPROACH

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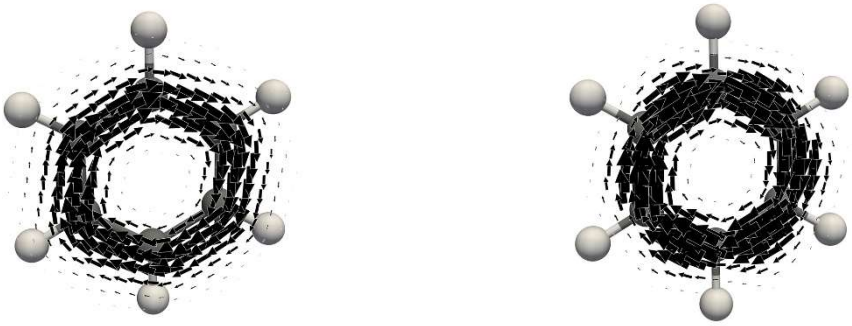
Calculations of the magnetically induced current densities represent a widely recognized approach for assessing the aromaticity and electron delocalization pathways in polycyclic conjugated molecules. From a historical perspective, Pople and McWeeny's extension of the Hückel–London theory was the first semiempirical method aimed at solving computational limitations in ring–currents modeling.[1,2] This study[3] examines the calculation of magnetically induced current densities within the CTOCD-DZ (Continuous Transformation of Origin of Current Density-Dimagnetic Zero) framework using various semiempirical methods based on the Neglect of Diatomic Differential Overlap (NDDO) approximation. The performance of these methods was assessed for a series of benzenoid hydrocarbons, by comparing their results with the B3LYP/def2-SVP reference. Additionally, it was proposed that the original NDDO-based semiempirical methods for calculating magnetically induced current densities be modified to further reduce computational costs while maintaining accuracy.



B3LYP/def2-SVP α-MNDO

Figure 1. π-electron current density maps plotted 1 Bohr above the molecular plane of benzene obtained using the B3LYP/def2-SVP and α-MNDO methods.

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THE P-ANIONIC CLAR STRUCTURES OF A FULLERENE

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A *fullerene* is a pure carbon molecule and corresponds with a 3-regular plane graph whose faces have degree 5 or 6. For a fixed integer p, a *p-anionic resonance structure* (F,M) of a fullerene G is a set of faces, $F \subseteq F(G)$, and a matching, $M \subseteq E(G)$, such that F contains exactly p pentagons (the remaining faces are hexagons) and each vertex of G is incident with exactly one element of FUM.

The *p-anionic Clar number* $C_p(G)$ of a fullerene G is the maximum value of $|F|$ over all possible p-anionic resonance structures for G. This parameter generalizes the Clar number and was introduced in [1]. This definition is motivated by the observation that in fullerene anions (negatively charged fullerenes), pentagons can compete with hexagons to host 'Clar sextets' of six electrons.

In this talk, we describe properties of p-anionic resonance structures in fullerenes, and show that the edges of M decompose into 'chains'. We introduce tools to find the p-anionic Clar numbers of fullerenes and find bounds on the p-anionic Clar numbers for families of highly symmetric fullerenes.

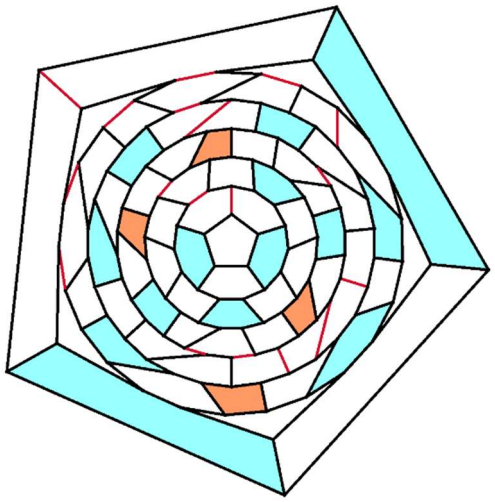

Figure 1. A 4-anionic resonance structure for an icosahedral fullerene with coordinates (2,1) between pentagons. Edges of M are red, pentagons of F are orange, hexagons of F are blue.

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WORKSHOP

CHALLENGES IN THE APPROACH TO MULTI-LEVEL SIMULATIONS OF ELECTRONIC STRUCTURE BASED ON FROZEN-DENSITY EMBEDDING THEORY

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The key idea of Frozen-Density Embedding Theory (FDET) was introduced in Ref. [1] and consists of using two independent variables for N_{AB} electrons in external potential v: Ψ_A – which has a structure of an N_A-electron wavefunction, and ρ_B - a non-negative real function integrating to an integer N_B such that $N_A+N_B=N_{AB}$. In multi-level simulation methods based on FDET, a N_A-electron eigenvalue equation is used to optimize Ψ_A for a fixed ρ_B, in which the external potential is modified by addition of the multiplicative operator (embedding potential). By construction, the FDET energy functional yields the energy of the whole N_{AB} electron system, which is equal to that given by the Hohenberg-Kohn energy functional ($E_v^{HK}[\rho=\rho^o_A+\rho_B]$), where ρ^o_A is the N_A-electron density obtained from the stationary solution of the FDET eigenvalue equation. For the exact relations between the Hohenberg-Kohn energy functional, the embedding potential, ρ^o_A, and ρ_B for various variational methods to treat electron correlation, see Ref. [2,3]. For non-variational methods, Ref. [4] gives the exact relations. FDET comncerns also excited states which correspond to ther then ground-state solutions of the FDET eigenvalue equation [5] or can be obtained from time-dependent response theory in case of Ψ_A being obtained for reference syytem of non-interacting electrons [6]. Practical applications of FDET hinge on availability of universal bi-functionals for the embedding potential and the corresponding component of the bi-functional for the FDET energy.

In the first part, we will introduce the FDET energy functional and the FDET eigenvalue equation, discuss and interpretat the involved quantities, and identify open questions related to this equation. The second part will concern development of approximants to the bi-functionals featuring in FDET and the relevant challenges. In the last part, illustrative applications of FDET based methods from us or from others will be shown.

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POSTERS

COMPUTATIONAL STUDY OF WEAK FORCE CONTRIBUTIONS TO RNA TETRALOOP STABILITY AND STRUCTURE

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RNA tetraloops are highly conserved structural motifs frequently found in RNA molecules. They typically cap RNA hairpins, which are among the most common secondary structural elements and play crucial roles as nucleation sites for RNA folding, as well as for RNA–RNA and RNA–protein interactions. Investigating the structural features of RNA tetraloops provides valuable insights into biological mechanisms associated with RNA tertiary structure. These motifs are generally compact, thermodynamically stable, and structurally conserved, and they often exhibit atypical interactions such as base–base, base–sugar, base–phosphate, and sugar–phosphate contacts[1].

Based on structural similarities, RNA tetraloops can be categorized into several distinct groups. In this study, we focused on the GNRA class—the most prevalent tetraloop group—where N represents any nucleotide and R denotes a purine[2]. We selected the crystallographic structure of an RNA segment containing a GNRA tetraloop (PDB ID: 1DUL) as our model system. The tetraloop, along with two flanking nucleotides on each side, was extracted from the full structure. Hydrogen atoms and counterions were then added and subjected to geometry optimization using Density Functional Theory (DFT).

To investigate the role of weak intramolecular forces, we applied the Independent Gradient Model based on Hirshfeld partitioning (IGMH) method[3]. We specifically analyzed three types of non-covalent interactions within the tetraloop: hydrogen bonds, π–π stacking interactions and C–H···O interactions. Our analysis enabled us to characterize, quantify, and visualize the weak forces that stabilize the three-dimensional conformation of the tetraloop[4].

Understanding how these weak interactions contribute to the structural integrity of RNA tetraloops offers deeper insight into RNA function and stability. The findings from this work provide a foundation for future studies on RNA tetraloops and their interactions with other biomolecules or xenobiotics.

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QUANTUM CHEMICAL RATIONAL DESIGN OF ORGANIC THERMOELECTRIC MATERIALS

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This work, part of the Pi-CANTHERM initiative, focuses on developing a rational design approach for n-type Organic semiconductors (OSCs) by integrating quantum chemical methods at both molecular and solid-state levels. Conjugated oligomers with alternating donor-acceptor units were investigated through conformational studies and DFT-based optimization in solution, identifying the most stable structures and their frontier orbital energies. Crystal structure prediction (CSP) was carried out using the Universal Structure Predictor: Evolutionary Xtallography "**USPEX"**[3-6], and candidate structures were further optimized using periodic DFT (DFT-PBC) as implemented in **CRYSTAL17**[1-2]. Our findings reveal that molecular conformation significantly affects HOMO-LUMO gaps, which range from 1.8 to 2.0 eV, and that the transition to the solid state reduces these gaps due to crystal field effects and geometric distortions. Moreover, different molecular packing motifs influence the band structure, with stacked arrangements leading to narrower gaps compared to glided packings. This multiscale computational approach provides valuable insight for designing efficient OSCs for thermoelectric energy conversion.

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NMR SPECTROSCOPY AND STATISTICAL ANALYSIS IN CHARACTERIZATION OF COMPLEX MIXTURES

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Detailed characterization of complex organic mixtures such as crude oils and wines is of a highest priority for their quality evaluation. The crude oil components are usually divided into four main groups: asphaltenes, saturates, aromatics and resins. Asphaltenes are the most complex crude oil components which can aggregate and precipitate during petroleum processing, causing different problems in crude oil industry. [1-3] Wine consists of 97 % water and ethanol, but each bottle of wine also contains large number of molecules, ranging from acids and sugars to phenolic compounds and low concentration aroma compounds. [4]

Many different analytical techniques and approaches were used to investigate properties and composition of such complex systems as crude oils and wines. [1] In this work it will be demonstrated that NMR spectroscopy is an indispensable tool for investigating complex organic samples. Although 1D NMR spectra of these types of mixtures consist of many overlapping signals, they still provide useful information on composition and structure. It will be demonstrated with several examples that ^{1}H and DOSY NMR techniques in combination with statistical methods such as principal component analysis and machine learning provide powerful approach to identify and classify crude oil samples of different origin. A model can be proposed for prediction of the crude oil stability as an essential parameter that affect oil properties, thus showing potential for practical applications. [3] Furthermore, it will be shown that a combination of experimental ICP-MS and NMR data and advanced tensor decomposition algorithms with *state-of- the-art* deep reinforcement learning procedures can provide a new and reliable classification model for the prediction of sparkling wines' geographical origin, especially in cases when other statistical methods such as cluster analysis fail. [4]

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DOES CHEM NEED MATH?

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The amount of mathematics needed to master chemistry can vary depending on the level of chemistry being studied and the specific area of focus.

I decided to find the answer to the question Does chemistry need mathematics? through conversations with students and through their answers and practical work so that they themselves understand the importance of interdisciplinary studies in STEM subjects.

20 students from 1st to 4th grade of high school participated.

In the first part of the work, students answered two questions through conversations:

- Why is chemistry so difficult for you?
- What are the branches of chemistry and how much mathematics do they involve?

The answers showed that students were aware of the need for mathematics in order to better understand the laws of chemistry.

In the second part, students prepared problem tasks and experiments in teams, along with explaining the necessary mathematical operations to solve them. Each team prepared one problem task and experiment, which they solved with other students.

Finally, the teams were tasked with finding tools on the internet to help them solve chemistry problems and experiments that require knowledge of mathematics.

In summary, math is essential for all levels of chemistry. As one progresses to college-level and specialized fields, knowledge of calculus and statistics becomes increasingly important. For a well-rounded understanding of chemistry and IT tools can help. Combination of all these skills is beneficial.

VISIBLE-LIGHT-ACTIVATED CO_2 PHOTOREDUCTION OVER CERIA-BASED HIGH-ENTROPY OXIDE CATALYSTS

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Up to this date, the development of highly efficient, visible−light−active catalysts remains a formidable challenge due to the enhanced rising of atmospheric CO_2 concentration.[1] This study discusses a class of ceria−based high−entropy oxides – designed to optimize charge carrier dynamics, surface reactivity, and CO_2 activation efficiency. Due to the advantages of high configurational entropy and multi−element synergy, these materials achieved improved photocatalytic performance, surpassing conventional ceria-based systems. Structural and spectroscopic analyses reveal that Pr^{3+}/Pr^{4+} redox pairs and abundant oxygen vacancies create an electronically disordered yet thermodynamically stable environment, which enhances charge separation and suppresses electron−hole recombination. Photocatalytic experiments demonstrated that $Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}O_{2-\delta}$ achieves the highest CO_2 conversion rate, reaching a conversion of 20.3% under visible-light irradiation, significantly surpassing pure ceria (1.4%), with a calculated STY of 10.15 $mol_{CO}kg^{-1}h^{-1}$ under the same conditions. First−principles density functional theory (DFT) simulations were employed to investigate the CO_2 reduction mechanism on CZLPS catalysts. The study elucidates the Gibbs free energy changes (ΔG) for each step of the reaction pathways leading to CO and HCOOH formation, highlighting the Zr site of CZLPS as the most active for CO_2RR, which is responsible for the outstanding catalytic activity.

Acknowledgements. This work has been supported by the Croatia-Israeli bilateral project entitled: High-Entropy Oxides Photoabsorbers for Efficient and Stable Photoelectrochemical Hydrogen Generation.

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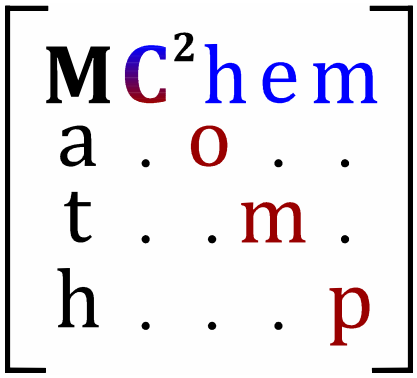

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