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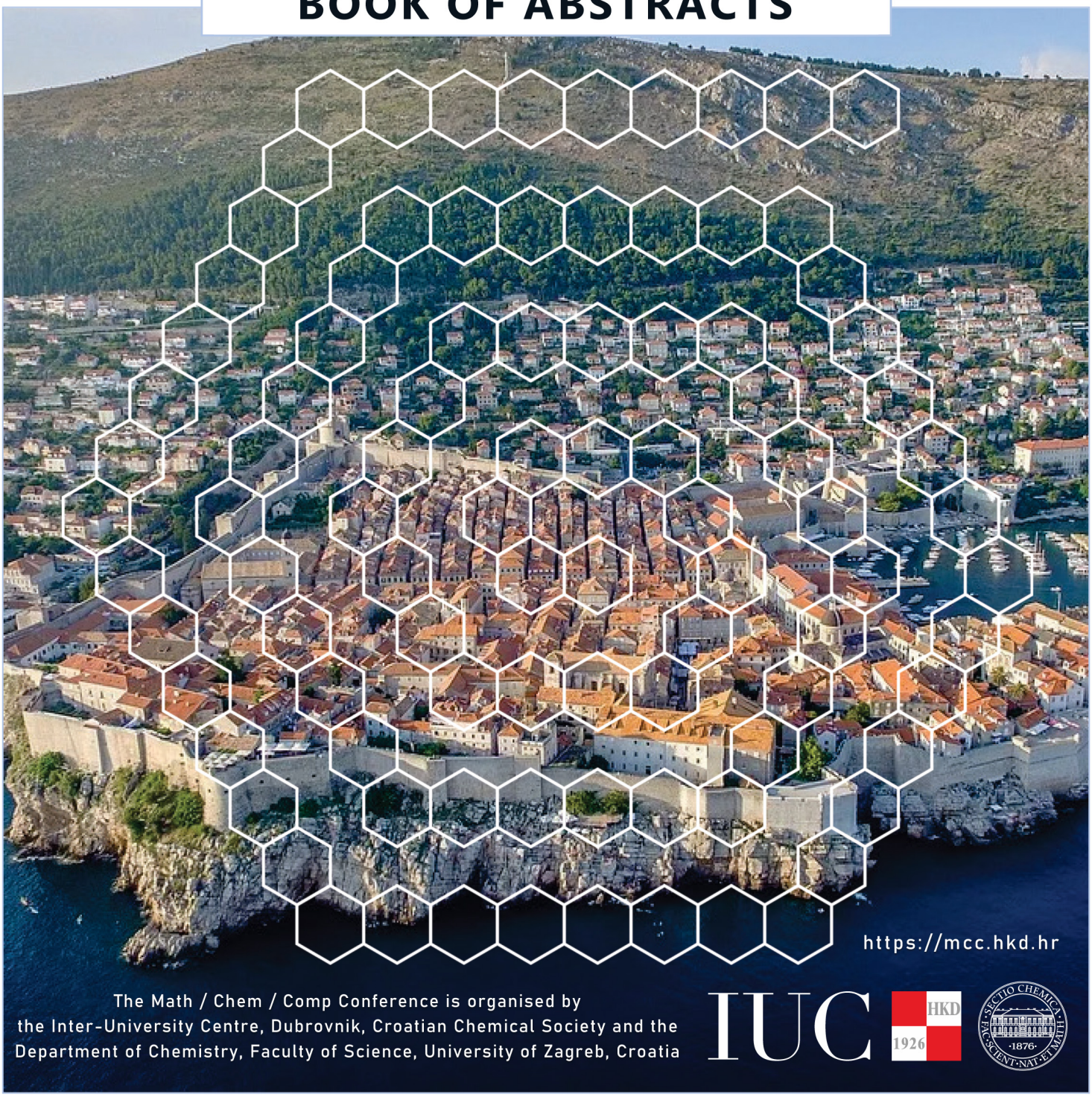
Math/Chem/Comp 2026 – 37th MC² Conference

Inter University Centre Dubrovnik, 1 – 5 June 2026

BOOK OF ABSTRACTS



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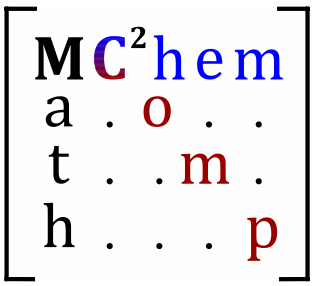

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IMPRESSUM

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The 37th International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences: Mathematics, Chemistry, Computing (Math/Chem/Comp, MC^2-37)

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^2-37 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**: "Organic reaction mechanisms – principles, interpretation, and generalization" which will be held by Professor Hrvoj Vančik, Department of Chemistry, Faculty of Science, University of Zagreb.

Proceedings

The papers presented at the MC^2-37 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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Inter University Centre Dubrovnik, 1 – 5 June 2026

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LECTURES

EXPLICITLY CORRELATED METHODS FOR SPECTROSCOPIC-ACCURACY CALCULATIONS IN HEH$^+$ AND HE_2^+

Mariusz Puchalski, Michał Siłkowski

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High-precision molecular calculations require a consistent treatment of electronic correlation, finite nuclear-mass effects, and higher-order relativistic and QED contributions across multiple spatial and energy scales. In this contribution, we present recent methodological developments in explicitly correlated approaches designed for spectroscopic-accuracy calculations in few-electron molecular systems. The presented framework combines variational explicitly correlated basis expansions with asymptotically adapted representations that enable stable treatment of competing correlation length scales over the full range of internuclear separations. Particular attention is devoted to the construction of hybrid variational spaces incorporating both fully correlated molecular sectors and separable asymptotic components, significantly improving numerical stability in the dissociation regime [1]. The methodology is demonstrated for molecular ions such as HeH$^+$ and He_2^+, which constitute important benchmark systems for precision spectroscopy, nonadiabatic theory, and molecular quantum electrodynamics. In particular, HeH$^+$, as the simplest heteronuclear two-electron molecular ion with unequal nuclear charges, represents a qualitatively different physical system from the isoelectronic H_2 molecule. The broken inversion symmetry, asymmetric dissociation channel, and strong coupling between different correlation and mass scales make HeH$^+$ a sensitive testing ground for high-accuracy treatments of nonadiabatic, relativistic, and QED effects at near-spectroscopic precision. The availability of high-resolution spectroscopic data further makes these systems particularly suitable for validating explicitly correlated computational frameworks [2,3].

The presented methodology provides a general framework for precision molecular calculations and can be extended to broader classes of molecular systems relevant to computational spectroscopy, molecular modeling, and mathematical chemistry.

Acknowledgements. This work has been supported by National Science Center (Poland) Grant No. 2019/34/E/ST4/00451

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ON-TOP TWO-ELECTRON DENSITIES COMPUTED WITH ONE-ELECTRON BASIS SETS AND THEIR (MIS)USE IN QUANTUM-CHEMICAL FORMALISMS

Jerzy Cioslowski

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The properties of the approximate on-top two-electron densities $\Phi(\mathbf{r})$ computed with one-electron basis functions are investigated in detail. The key findings of these investigations, which also concern the reduced variant of $\Phi(\mathbf{r})$, i.e. $4\,\Phi(\mathbf{r}) / \rho(\mathbf{r})^2$ [where $\rho(\mathbf{r})$ is the one-electron density], are as follows: 1) $\Phi(\mathbf{r})$ converge extremely slowly to the complete basis set (CBS) limits, their errors asymptotically scaling like $N^{-1/3}$ with the number N of basis functions (as contrasted with the N^{-1} error scaling of the electronic energy); 2) this slow convergence results in gross inaccuracies of the approximate $\Phi(\mathbf{r})$ computed with standard basis sets; 3) the errors in these $\Phi(\mathbf{r})$ are in general refractory to reduction with standard convergence acceleration techniques such as the CBS-limit extrapolation; 4) it is essential to make a distinction between the physically meaningful genuine $\Phi(\mathbf{r})$ (such as those produced by highly accurate calculations) and the contrived ones (such as those appearing in some variants of the Kohn-Sham formalism and in overly simplistic models) that are merely auxiliary quantities to which no physical meaning should be attached; 5) due to the presence of spurious features in the contrived $\Phi(\mathbf{r})$, their employment in analysis of electronic structure leads to false and misleading conclusions on chemical bonding and electron correlation; and 6) the MC-PDFT formalism suffers from a hidden ''double-counting'' problem whose presence is masked for sufficiently small active spaces by its use of the contrived $\Phi(\mathbf{r})$.

DENSITY MATRIX CHANGES IN MOLECULAR INTERACTIONS

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When two molecules are close, their electronic densities fluctuate and deform in response to one another. Although small, these changes drive many physical, chemical, and biological phenomena, including collision-induced absorption in molecular spectra, molecular-crystal formation, and ligand–protein binding. Here, we investigate electron-density changes in selected model systems representing different van der Waals interactions, including hydrogen bonding, σ-hole bonding, atom…atom contacts, and dispersive stacking.

We use propSAPT, an innovative variant of symmetry-adapted perturbation theory developed by our group for molecular-property calculations. The method expresses interaction-induced electron-density changes as perturbative corrections in orders of the interaction operator and has previously been applied to interaction-induced properties such as dipole moments.[1] In propSAPT, density corrections naturally decompose into polarization, exchange, and dispersion contributions, analogous to the standard SAPT energy decomposition. This enables physically transparent analysis and visualization of noncovalent-interaction-induced density shifts. We compare propSAPT differential densities with supermolecular coupled-cluster results and contrast dispersion-driven density changes with those from the MBD@FCO many-body dispersion model based on quantum Drude oscillators.[2]

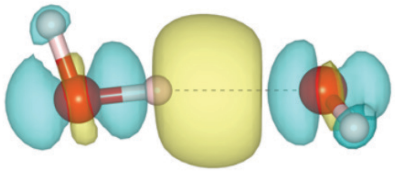

Figure 1. Electron density changed induced by dispersion interaction in water dimer

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

Henryk A. Witek,[a] Meng-Han Wu,[a] Grzegorz Pestka,[b] Anjan Sadhukhan,[a] Rafal Podeszwa[c]

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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 associated with each of these operators. This identification allows us to reduce the dimentionality of the wave function by eliminating those degrees. 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 a family of reduced Schrödinger equations 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, its projection M, and parity π. The derived formalism is used to compute very accurate energy levels of a few-particle systems.

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ELECTRIC FIELD GRADIENT: BRIDGING EXPERIMENT AND COMPUTATIONS

Valera Veryazov,[a] Marek Krośnicki[b]

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Atomic structures are often treated as known quantities, obtained either from experiment or from computation. In some systems, however, this assumption breaks down. Th-doped CaF_2, relevant for nuclear clock applications, is one such case: the local environment of Th remains poorly characterized despite significant experimental and theoretical effort. Total energy considerations alone are insufficient to resolve competing structural models, particularly in the presence of charged defects and ambiguous chemical compositions.

In this work, we explore the use of electric field gradients (EFG) as an alternative, highly sensitive probe of local structure. Combining embedding cluster models with high-level wavefunction methods (CASSCF/CASPT2), implemented in Molcas [1], we show how EFG can provide direct insight into local symmetry and serve as a stringent test of computational models. **We also discuss key mathematical properties of the EFG tensor—such as its traceless property, symmetry, and sensitivity to small perturbations—which underlie its usefulness as a structural probe.** We further highlight a less obvious issue: different implementations of EFG may differ by sign due to convention, leading to systematic discrepancies across codes. Understanding and resolving such subtleties is essential when bridging experiment and computation. Finally, the EFG values can be used for quality control for various embedding models [3].

Acknowledgements. This work has been supported by Polish National Agency for Academic Exchange under the Strategic Partnership Programme grant BNI/PST/2023/1/00013/U/00001, eSSENCE@LU 11:2, and grant WISE-WASP-02-05.

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TOPOLOGY, AROMATICITY, AND GROUND-STATE STABILITY IN INDENOFLUORENE FRAMEWORKS

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Conjugated polycyclic hydrocarbons (CPHs) have gained considerable interest due to their versatile applications in optoelectronic devices, organic spintronics, and semiconductors, as well as energy storage devices. Among such CPHs, conjugated indenofluorenes (IFs) possess one of the most interesting topologies of delocalized π-electrons with different types of behavior (aromatic/antiaromatic) and ground state electronic structure (biradical/quinoidal). They exhibit a 6-5-6-5-6 ring architecture, which is obtained by a fusion of the indene unit to various positions of the fluorene unit to generate five possible isomers. In this work, the Ground State Stability (GSS) rule is introduced. It allows predicting the nature of the ground state of indenofluorene (IF)-type systems from the simple counting of the Clar π-sextets in the closed- and open-shell configurations.[1] Then, the molecular and electronic structure of the non-alternant indeno[2,1-b]fluorene system is examined using density functional theory and high-level *ab initio* calculations. Our results reveal the existence of a flat potential energy surface (PES) with a bond-localized C_s structure and a more delocalized, mirror-symmetric C_{2v} structure.[2] Depending on the level of calculation, the latter is a minimum on a single-well PES or a transition state connecting two C_s structures in a double-well PES. The change of the PES can also be modulated with substituents.[3]

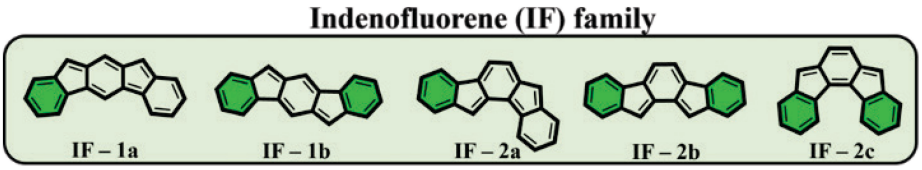

Figure 1. The five members of the indenofluorene family

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WHY ARE THE EXCITED STATES OF HETEROCYCLES STILL CHALLENGING FOR THEORY?

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Heterocyclic compounds are essential building blocks of biomolecules and systems that are highly relevant for optoelectronic applications. Surprisingly, even the lowest electronically excited states of heterocycles present a challenge for quantum chemical calculations.[1] This arises from the difficulty of providing a balanced description of excited states with very different characters, e.g., bright vs. dark, ionic vs. covalent, singly vs. doubly excited, etc. We analyse the origins of these excited state dichotomies from both molecular orbital and valence bond theory perspectives, using pseudosymmetry arguments that connect the two viewpoints.[2] We discuss the importance of electronic correlation for achieving a balanced description of excited states and explain why it is difficult, or even impossible, to reach high accuracy with conventional density-functional theory approximations. Finally, we delve into the origins of a less studied but recurring problem of valence-Rydberg mixing.

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SOLVATION ENERGIES VIA MACHINE LEARNING WITH PHYSICALLY SOUND FEATURES

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We have proposed a family of artificial neural network methods for calculating solvation free energy ΔG°_{solv} of molecules and ions based on physically sound input features. An early version of the method, *ESE-EE-DNN*,[1,2] uses *COSMO*[3] electrostatic energy, atomic cavity surface areas, total cavity volume, and induced surface charges as input features. For the electrostatic calculation, a specially modified version of electronegativity-equalization atomic charges is employed. A more efficient method, *ESE-GB-DNN*,[4] avoids an explicit cavity construction by using generalized-Born terms, as well as atomic surface areas and the molecular volume. A slightly modified version of *ESE-EE-DNN*, dubbed *ESE-ΔH-DNN*,[5] yields both ΔG°_{solv} and ΔH°_{solv} for neutral solutes. The newest method of the ESE-DNN family, *AtomicESE* [6], calculates ΔG°_{solv} by summing atomic contributions $\Delta G^\circ_{solv}(i)$ for each atom i, with each $\Delta G^\circ_{solv}(i)$ evaluated by a dense neural network. This atomic network uses six local atomic features, two global charge-related molecular properties, and five solvent-specific properties. For neutral solutes, AtomicESE achieves an average RMSE for organic solvents below 0.6 kcal/mol, demonstrating strong performance across diverse classes of organic solvents.

To further improve the performance of the solvation-energy schemes, we introduced an atomic-charge scheme, *BoostCha*,[7] based on Gradient Boosting Decision Trees. The *BoostCha* model predicts pseudo-charges for individual atoms from their local environments, represented by 3-D Kocer–Mason–Erturk descriptors. The BoostCha charges are employed as input features in two independent machine-learning models for predicting solvation free energies in organic solvents: *ESE-Boost*, a gradient-boosting model, and *ESE-ANN*,[7] a dense artificial neural network. Both approaches yield robust and consistent predictive performance, with average RMSE of about 0.5 kcal/mol.

Acknowledgements. This work has been supported by the Spanish Ministerio de Ciencia, Innovación y Universidades (grant PID2023-147424NB-I00).

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ACCELERATING QUANTUM-CHEMICAL MULTILIGAND SIMULTANEOUS DOCKING WITH DEEP REINFORCEMENT LEARNING

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This study employs quantum-chemical multiligand simultaneous docking (MLSD) to identify potent single or joint inhibitors of human acetylcholinesterase (hAChE), human butyrylcholinesterase (hBChE), and/or equine butyrylcholinesterase (eqBChE). Moving beyond traditional single-molecule docking, we adopted a fragment-based paradigm, docking multiple small molecular scaffolds designed for subsequent assembly *via* modular organic synthesis. To navigate the high-dimensional configurational space and the computational complexity associated with translational, rotational, and conformational degrees of freedom, we developed a parallelized Monte Carlo algorithm to enhance sampling efficiency.[1] This framework incorporates a smart structure generator for pre-screening and input optimization. Binding enthalpies were determined using the PM7 semiempirical Hamiltonian,[2] which has been shown to outperform other semiempirical methods for organic molecules.[3] To overcome the computational bottleneck of PM7 calculations, particularly in multiligand systems, we integrated deep neural networks (DNNs) trained on-the-fly *via* deep reinforcement learning.[4] These DNNs accurately approximate potential energy surfaces (PESs), substantially reducing the computational cost of energy determinations. Finally, active-site coverage was monitored dynamically throughout the simulations using probability density functions to ensure optimal ligand placement throughout the active site.

Acknowledgements. This work was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-9525.

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CATALYTIC REACTION MECHANISTIC MULTI-SCALE MODELLING SIMULATIONS: LINKING ATOMS–CONTINUUM

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Catalytic reaction mechanistic multi-scale modelling has emerged as a powerful simulation framework for bridging the atomic scale chemistry with industrial continuum level reactor, separator and process behaviour. At electronic, atomistic and molecule modelling levels, first principles calculations, density functional theory and *ab initio* molecular dynamics' simulations provide a fundamental mechanistic insight into surface adsorption energetics, reaction pathways, transition states, structure–activity relationships and selectivity dependence of homogeneous or heterogeneous catalytic materials. These form the basis for micro-kinetics that captures the intrinsic reaction rates/mechanistic selectivity under realistic operating conditions. Beyond isolated active sites, mesoscale accounts for morphology, heterogeneity, and transport. Coupling the micro-kinetics with transport phenomena resistances enables the prediction of the non-isothermal heat effects, mass transfer resistances and chemical concentration gradients across heterogeneous catalyst particles, beds and electrodes. In reactors/processes, models integrate thermodynamics, transport and dynamics to assess performance, efficiency and scalability. Advances demonstrate the integration of the insights into the macroscale for thermo-catalysis, electrochemistry and photo-catalysis, including hydrogen carrier cycles, CO_2 reduction and nitrogen. Such mechanistic, hierarchical and concurrent multi-scale modelling approaches enable rational catalyst design, industrial process optimization and techno-economic technology assessment. Despite progress, challenges remain in efficiency, uncertainty and transferability. A continued computational development of mechanistically consistent multi-scale modelling frameworks is essential for predictive catalysis screening, the accelerated scalable deployment of technologies and digitalisation.

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QUANTUM-MECHANICAL PROTOCOLS FOR DECODING LIGHT–MATTER INTERACTIONS

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Molecular systems of increasing size and complexity from small prebiotic molecules of astrochemical interest [1,2], medium size chromophores important for technology applications [3] to larger bio-molecules such as proteins [4,5] are nowadays studied by broad range of experimental techniques, involving different parts of electromagnetic spectrum [6], as depicted in Figure 1. However, it is seldom straightforward to link the rich experimental data to the desired information on the specific structure and properties of complex molecular systems.

I will discuss status and perspective of the project aimed at development, validation and application of QM based computational protocols supporting to decode and analyze experimental data based on light-matter interaction.

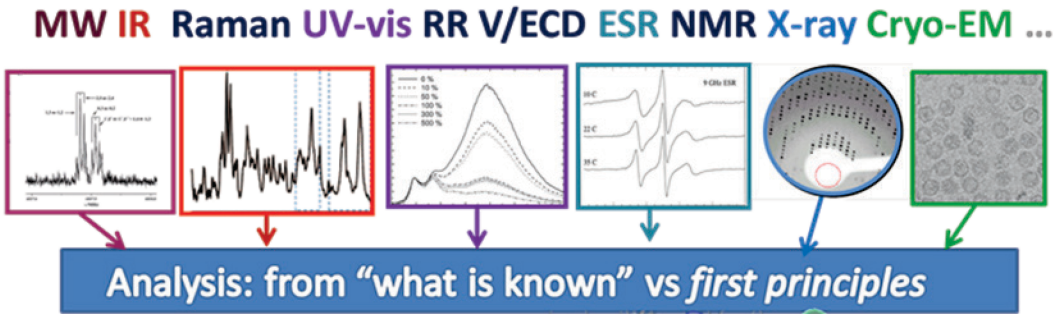

Figure 1. First principles support for experiments.

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GRAPHS MAXIMIZING THE GENERALIZED COMPLEMENTARY SECOND ZAGREB INDEX

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The complementary second Zagreb index exhibits strong correlations with physicochemical properties and effectively models the heat of vaporization, particularly its normalized form, in compounds such as octanes and benzenoid hydrocarbons. We confirm a conjecture by Furtula and Oz [1] concerning graphs that maximize the second complementary Zagreb index.[2] We further extend this result to a broader class of parameter-dependent indices, which we term the *generalized complementary second Zagreb index*. We prove that all indices within this class attain their maximum on complete split graphs. Additionally, we analyze the behavior of the clique order in extremal graphs [2,3]. For the classical second complementary Zagreb index, we derive an explicit formula for the maximum value, thereby confirming the conjectured result of Furtula and Oz [1].

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A NEW DESCRIPTION OF MOLECULAR CONSTITUTION: FROM PLATONIC SOLIDS TO MOLECULES

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Chemical graph theory is a branch of science that connects mathematical topology with chemical structural theory. It is applied to study the relationships between the main components of molecular structures: the number of vertices, the number of edges, and the number of rings in polycyclic molecules. These relationships form the basis of the IUPAC nomenclature for polycyclic hydrocarbons. To some extent, this approach is a corollary of Euler's formula regarding the number of vertices, edges, and faces.

However, to gain deeper insight into the problem of molecular structure - particularly the relationship between molecular constitution and configuration - the graph theoretical approach to polycycles has been expanded with new definitions of rings and bridges. This expansion simplifies the enumeration of edges and vertices: the number of edges is now the sum of the number of bridges and the number of vertices.

It is demonstrated how this approach is generally valid and how it provides additional knowledge about molecular complexity.

IMPROVING RELIABILITY OF PROTEIN FOLDING RATE PREDICTIONS USING SEQUENCE AND STRUCTURAL INFORMATION

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Protein folding is regarded as an extremely important problem in the life sciences, chemistry, and biophysics, and has been intensively studied for many years both experimentally and through modelling.[1] It is assumed that all key information related to the process and rate of protein folding is contained in the primary structure of the protein. Over the past 30 years, the dependence of protein folding rate k_f (s^{-1}), defined as $k_f = 1/t_f$ (where t_f is the folding time) has been intensively modelled. Among the most important structural descriptors related to protein folding rate are protein length, the content of regular secondary structures, and the topology and average contact order distance between amino acids in the 3D structure have been identified as the most significant.[2] We conducted comparative studies of different methods for predicting protein folding rates, available as web servers and from the literature, and compared the results with those of a previous study.[3] We found that experimental data in literature databases and data available online are inconsistent and scattered. We also identified errors in the method evaluation in a previous, highly influential study.[3] After making the necessary corrections, we developed simple models for predicting protein folding rates based on the length of the protein chain. These simple models, in several comparisons, showed greater stability in prediction than almost all existing models from the literature. In addition, we proposed a physicochemical interpretation for these models with respect to transition state theory and polymer chemistry theory.[4]

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LEARNING-BASED METHODS FOR IMAGE QUALITY IMPROVEMENT IN COMPUTATIONAL TOMOGRAPHY

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Improving image quality while reducing radiation exposure remains one of the central challenges of modern computational tomography. In particular, noise reduction constitutes a fundamental problem closely connected to mathematical modeling, inverse problems, and computational reconstruction algorithms. Alongside conventional analytical and iterative approaches, learning-based image enhancement methods have recently become increasingly important.

In this presentation, we introduce several deep learning architectures developed for noise suppression and image quality improvement in computational tomography. Special emphasis is placed on the underlying mathematical and physical modeling of the imaging process, including the simulation of realistic noise generation in a multi-slice cone-beam tomography system. The proposed approaches employ supervised learning strategies trained exclusively on mathematically generated phantoms with artificially simulated physical noise.

The work combines techniques from applied algebra, computational mathematics, mathematical physics, and machine learning, illustrating the interplay between data-driven methods and physically grounded modeling. The effectiveness of the proposed methods is demonstrated on both synthetic phantom data and real tomographic measurements, showing substantial improvements in reconstruction quality and robustness.

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MULTIPLE DAVYDOV *ANSÄTZE* AS SOLUTIONS TO LINDBLAD MASTER EQUATIONS

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Lindblad master equations describing driven quantum systems coupled to multiple bosonic modes are central to modeling cavity quantum electrodynamics and pseudomode models. In this work, we employ the density-operator-based Dirac–Frenkel time-dependent variational principle combined with the multiple Davydov D_2 Ansatz to provide optimal solutions for Lindblad master equations in both multimode and driven scenarios. Our approach is benchmarked against numerically "exact" methods in two representative models. The first describes a driven qubit subject to spontaneous emission and coupled to a lossy cavity, while the second corresponds to the pseudomode Lindblad master equation derived from the driven spin-boson model, incorporating seven discrete pseudomodes. The proposed variational approach achieves excellent agreement with numerically "exact" results. Furthermore, we analyze the accuracy of the variational solutions using an error metric based on the Frobenius norm, confirming their reliability. Overall, the present method offers an accurate and computationally efficient framework for simulating Lindblad master equations in complex open quantum systems.

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"MWK" MODEL OF CONFINED NANOSYSTEMS

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The relationship between the reaction constant and the quantum properties of the reactants is a topic at the border between chemical kinetics and quantum mechanics. The reaction constant, usually denoted by k, characterizes the rate at which a chemical reaction occurs; it depends on factors such as temperature, the nature of the reactants, and the activation energy; in the transition state theory, this constant is related to the formation of the activated complex. On the other hand, in the quantum description of particles, the state of motion is characterized by the wave vector k, which is directly related to the momentum by the relation; this concept arises naturally in the theory of quantum scattering, where chemical reactions are treated as collision processes between particles. The present work explores the connection between the reaction constant and the wave vector. Thus, in elementary gas-phase processes, the reaction constant can be expressed as the product of the relative velocity of the particles and the effective reaction cross section. Since the velocity is related to k, and the effective cross section is a function of it, it follows that k-"rate reactions" becomes a function of k – "wave vector", and, although not identical, they are in a functional relationship "k (rate reactions) ~ k (wave vector)"). Even in extreme conditions, such as very low temperatures or ideal quantum systems, this relationship remains of interest. In this new conceptual context, the new relationship as $\Delta m \sim \omega k$ ("MWK" Model) describes a proportional relation between mass change in a nanosystem and the rate constant of a chemical process occurring on its surface. Further quantum Einstein-Planck-De Broglie considerations produced the working quantum-relativistic connection under the momentum form $\hbar = \alpha c\sqrt{p}$ allowing to correctly describing the quantum-system scale factor $[\alpha] = kg^{1/2}m^{1/2}s^{1/2}$; moreover it becomes a quantum length–action hybrid scale $\alpha_{system} = \sqrt{m^*_{carrier} \cdot L_{conf}}$ that encodes effective mass $m^*_{carrier}$ of the relevant carrier (e.g. electron, exciton, proton, quasiparticle), and the characteristic coherence length scale L_{conf} (e.g. MOF pore size, tunneling distance, active exciton length site size) in nanosystems. The study of these relationships contributes to the development of nanotechnology and a better understanding of chemical and biochemical processes at the (sub)microscopic scale, e.g. enzyme nanokinetics (understanding reaction rates in confined biological environments), nanoreactors (designing systems where reaction rates are maximized under unity conditions), quantum biology (exploring wave effects in biochemical processes), or biosensing (interpreting signal generation at low molecular numbers). Relevant numerical examples are correspondingly given.

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OPEN QUANTUM SYSTEMS DRIVEN BY CHIRPED PULSE: QUANTIZED VS. SEMICLASSICAL FIELD & THE VALIDITY OF RWA

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Population transfer via chirped rapid adiabatic passage is studied using open quantum and semiclassical models, with and without the rotating-wave approximation. A time-dependent variational approach based on the multiple-Davydov D_2 trial state is employed to simulate the quantum models with an arbitrary finite mean photon number. We examine the accuracy of both the semiclassical field description and the rotating-wave approximation. Robust population transfer is identified over a wide parameter regime controlled by the laser spectral chirp and is found to be insensitive to the spin–phonon coupling strength, Gaussian pulse area, and energy gap of the two-level system.

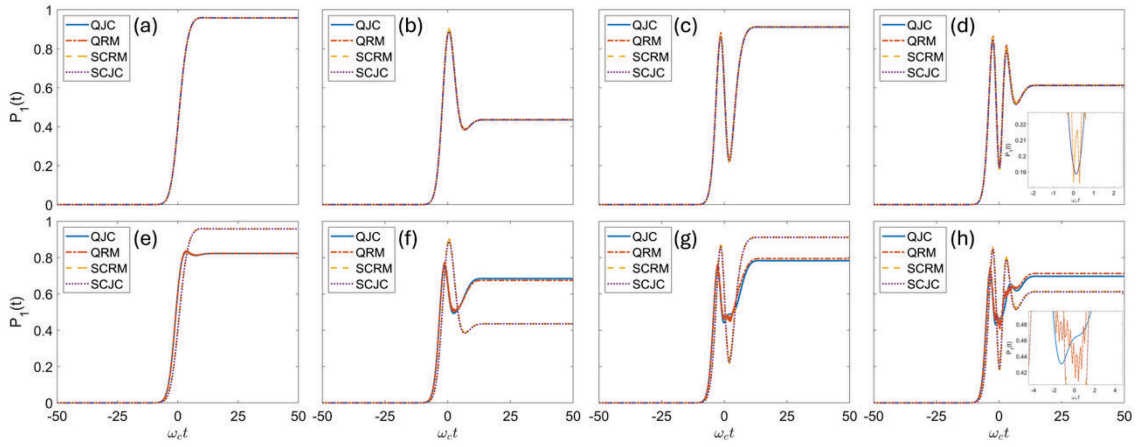

Figure 1. Time evolution of population transfer $P_1(t)$ of the quantum JC model (blue), quantum Rabi model (orange), semiclassical Rabi model (yellow) and semiclassical JC model (purple) with different initial mean photon number $|\alpha|^2$ for various pulse area: (a) $|\alpha|^2 = 10^4$, $\Theta = \pi$; (b) $||\alpha|^2 = 10^4$, $\Theta = 2\pi$; (c) $|\alpha|^2 = 10^4$, $\Theta = 3\pi$; (d) $|\alpha|^2 = 10^4$, $\Theta = 4\pi$; (e) $|\alpha|^2 = 1$, $\Theta = \pi$; (f) $|\alpha|^2 = 1$, $\Theta = 2\pi$; (g) $|\alpha|^2 = 1$, $\Theta = 3\pi$; and (h) $|\alpha|^2 = 1$, $\Theta = 4\pi$. The spin-phonon coupling A is set to be $0.22\omega_c^{-2}$, the spectral chirp $\varphi'' = -7\ \omega_c^2$ and the energy gap at resonant excitation ($\varepsilon = \omega_0$) is set at 10 ω_c.

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WORKSHOP

ORGANIC REACTION MECHANISMS – PRINCIPLES, INTERPRETATION, AND GENERALIZATION

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Chemistry, particularly organic chemistry, is the science dedicated to studying the properties and transformations of matter. Following the advancements in the determination of structures and synthesis of organic compounds, there was a significant surge in research at the end of the 19th century and throughout much of the 20th century. This research increasingly focused on understanding chemical reactions.

Key questions arise from this interest: How is the structure of the starting compounds linked to their potential transformation into specific products? To what extent can the theories of chemical kinetics, which originated in physical chemistry, be applied to predict the rates of organic reactions and the molecular structures of the resulting products? Furthermore, what defines chemical reactivity, and what contributes to the stability of organic molecules? How can quantum theory elucidate the nature of chemical reactions based on electron structure?

These inquiries and others have propelled the development of a subdiscipline that has evolved from the mid-20th century to the present day: the theory of organic reaction mechanisms.

POSTERS

UNIVERSALLY APPLICABLE RANGE-SEPARATION TUNING

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Range-separated hybrid functionals that employ approaches such as "*ionization-energy tuning*" or "*optimal tuning*"[1,2] of the screening parameter have emerged as highly accurate and reliable tools for describing excited-state phenomena across a broad range of systems, including condensed-phase materials. Despite their success, these methods typically rely on iterative self-consistent procedures that are computationally expensive and can suffer from convergence instabilities, particularly for large and complex systems.

In this study[3], we introduce a simple yet efficient alternative for determining the screening parameter, based solely on the total electron density of the system and the density functional theory (DFT) compressibility sum rule. The proposed framework provides remarkable accuracy, especially for charge-transfer excitations, surpassing the performance of previously developed approaches[4].

Because the method depends exclusively on the electron density, it possesses a transparent theoretical foundation and can be seamlessly integrated into automated DFT workflows for complex molecular and bulk materials, where conventional tuning strategies often become impractical. Furthermore, the approach serves as a promising starting point for single-shot Green's function methods such as G_0W_0 and the Bethe-Salpeter Equation (BSE)[5]. It also opens new avenues for the rational design of advanced organic photovoltaic materials, delivering predictive accuracies approaching those of CCSD(T) and many-body Green's function techniques[6].

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PROTOCATECHUIC ALDEHYDE AS ANTIOXIDANT AND PROOXIDANT

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Protocatechuic aldehyde is a natural compound that can be found in various plants, food, some algae and herbs[1]. It has been a subject of scientific research due to its positive effects on health. For example, this compound shows antioxidant[2-4] and anticancer activity[1,5], cardioprotective effect[6], to name a few. The anti- and prooxidant potency of protocatechuic aldehyde was evaluated using DFT approach (SMD/M06-2X/6-311++G(d,p), physiological conditions, aqueous and lipid environments). The focus was on thermodynamics and kinetics of direct scavenging of hydroperoxyl and lipid peroxyl radicals (single electron transfer and formal hydrogen atom transfer); on the repair of oxidative damage in biomolecules; and on the prooxidant ability of phenoxyl radicals. Additionally, sequestration of catalytic ferrous and ferric ions was studied, and molecular docking was used to study the inhibition of xanthine oxidase. The obtained results indicated studied compound as multifunctional antioxidant, due to its capability to scavenge studied radicals, repair damaged biomolecules, chelate iron ions and inhibit enzyme activity.

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VISIBLE-LIGHT-ASSISTED REDUCTION OF CARBON DIOXIDE CATALYZED BY ORDERED AND DISORDERED CERIA-ZIRCONIA-BASED STRUCTURES

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Ceria-zirconia-based oxides are widely recognized as efficient redox catalysts due to their exceptional oxygen storage capacity (OSC) and the facile interconversion between Ce^{3+} and Ce^{4+}, which enables dynamic generation of oxygen vacancies, an important feature in various types of catalysis. We extend this concept by introducing configurational entropy through the synthesis of rare-earth high-entropy ceria-zirconia oxides and systematically compare them with their ordered and partially ordered binary counterparts. A series of solid solution, pyrochlore, kappa, and partially oxidized phases were prepared via a controlled aqueous citrate sol-gel route followed by redox-driven structural transformations. Comprehensive structural and surface characterization revealed that entropy-stabilized materials exhibit pronounced lattice distortion, enhanced defect tolerance, and a higher density of redox-active surface sites. Spectroscopic analyses demonstrate that high-entropy pyrochlore-derived phases possess abundant oxygen vacancies, surface hydroxyl groups, and stabilized mixed-valence Ce and Pr centers, which collectively promote efficient charge separation and surface reactivity under visible-light irradiation. Despite nominal band gap values exceeding 3 eV, UV-Vis-NIR and XPS measurements confirm visible-light activity arising from multiple electronic transitions induced by multication disorder. Density functional theory calculations provide direct insight into the role of entropy and structural order on CO_2 activation, showing that high-entropy surfaces exhibit favorable CO_2 adsorption energies while maintaining comparatively weak CO binding, thereby minimizing product poisoning and sustaining catalytic turnover. Photocatalytic CO_2 hydrogenation experiments under visible light reveal that pyrochlore-fluorite dual-phase and partially oxidized pyrochlore high-entropy oxides achieve the highest CO_2 conversion of 24.15 % and 21.77 %, respectively. Although all catalysts showed selectivity for CO, the selectivity for formaldehyde formation was only achieved for these two types of compounds with the values of 10.02 % and 5.22 %.

UNCOVERING THE BINDING MECHANISM OF UGI-DERIVED PEPTIDOMIMETICS TO BUTYRYLCHOLINESTERASE

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Butyrylcholinesterase (BChE) is a primary therapeutic target for the treatment of Alzheimer's disease,[1,2] yet the complexity of its active site necessitates precise modeling of ligand-protein interactions to develop effective inhibitors. This study proposes a "bottom-up" design strategy for novel inhibitors by utilizing the versatility of the multicomponent Ugi reaction (UGI). To ensure that the resulting UGI products possess high binding affinity and optimal fit, we employed quantum-chemical semi-flexible molecular docking[3] to model the precise spatial placement of individual UGI reactants within the equine BChE active site. This fragment-based approach allows evaluation of how individual building blocks interact with the enzyme's electronic environment prior to their covalent assembly. Our results indicate that although individual components exhibit modest IC50 values, the specific spatial orientation of formaldehyde and benzylamine relative to the catalytic triad suggests strong synergistic potential. By analyzing these interactions, we provide a theoretical foundation for the synthesis of both three-component UGI products[4] (utilizing an amine, aldehyde, and isocyanide) and four-component UGI products[5] (incorporating an additional carboxylic acid), an insight particularly valuable for the rational selection of precursors to further tune the molecule's polarity and binding. This strategy highlights the distinct advantage of UGI chemistry: the ability to rapidly assemble complex, drug-like molecules that are pre-optimized for the BChE binding pocket, thereby significantly reducing the trial-and-error phase of lead optimization.

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IN SILICO SCREENING OF IMIDAZOLIUM CATIONS AS FUNGAL CHITINASE INHIBITORS

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Imidazole derivatives are important compounds in heterocyclic chemistry due to their diverse biological activities, which have led to the development of many commercial drugs and pesticides. Imidazolium-based ionic liquids, characterized by favorable physicochemical properties, have also demonstrated antimicrobial activity and are considered as adequate drug candidates. However, their application in the field of plant protection remains limited.[1] As nitrogen-containing heterocycles, imidazolium-based ionic liquids may serve as effective antifungal agents against phytopathogens by disrupting the integrity of fungal cell walls and membranes.[2] This study aimed to perform a preliminary in silico screening of imidazolium cations with varying side chain lengths to evaluate their potential binding to fungal chitinase. Chitin, a key structural component of fungal cell walls, is degraded by chitinases during cell wall remodeling. Thus, inhibition of this process may compromise fungal cell viability.[3] A series of eight imidazolium cations with side chains ranging from 0 to 12 C atoms was designed, exhibiting increasing lipophilicity with chain length. Following structural optimization, molecular docking was performed on chitinase B (a bacterial-type enzyme found in fungi). As expected, cations with longer side chains generally showed more favorable docking scores, likely due to increased van der Waals interactions. Notably, the imidazolium cation with a side chain of 6 C atoms exhibited the highest binding affinity, with a total energy of –75.9 kcal mol^{-1}. All compounds interacted with at least one active site residue and were positioned near the substrate binding site. These results provided a valuable insight for further design of imidazolium cations as fungal chitinase inhibitors.

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IN SILICO INVESTIGATION OF ANTIFUNGAL MECHANISMS OF ACTION FOR 1,2,3-TRIAZOLE–COUMARIN DERIVATIVES

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Fungi are among the main food contaminants, affecting both organoleptic properties and consumer safety. Among these, *Aspergillus flavus* has become an increasing concern in Europe in recent decades, primarily due to its rising prevalence in agricultural commodities and its ability to produce aflatoxins, which are highly toxic and carcinogenic secondary metabolites [1]. Strategies to control *A. flavus* commonly rely on fungicides; however, this approach is increasingly limited by the progressive withdrawal of some of the most effective compounds due to their toxicological risks. In the search for novel antifungal agents against *A. flavus*, five 1,2,3-triazole–coumarin derivatives were selected for synthesis based on their favourable ADMET properties and pesticide-likeness profiles. Their potential antifungal mechanisms of action were investigated by molecular docking against two enzymes involved in sterol biosynthesis: squalene synthase and sterol 14α-demethylase. All five compounds exhibited the expected interactions with the haem cofactor of sterol 14α-demethylase, predominantly through π-π interactions involving the coumarin moiety. Intramolecular π-π interactions between aromatic rings within the ligands were also observed. Docking analysis of squalene synthase also yielded promising results, with all compounds interacting with amino acid residues in the enzyme's active site. Collectively, these findings suggest that the investigated compounds may act as dual inhibitors of key targets in fungal sterol biosynthesis. Nevertheless, these preliminary results require further computational and experimental validation.

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QUANTUM-CHEMICAL DOCKING OF FOUR-MEMBERED RINGS IN THE ACTIVE SITE OF BUTYRYLCHOLINESTERASE

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The progression of Alzheimer's disease is characterized by the increasing relevance of human butyrylcholinesterase (hBChE) as a therapeutic target.[1] However, achieving high pharmacological selectivity for hBChE remains an enduring challenge. In this work, we explore the potential of small four-membered heterocyclic rings as modular building blocks for the design of next-generation hBChE inhibitors, employing a fragment-based computational approach. To elucidate the binding of these fragments, we developed a docking workflow based on quantum-chemical calculations. The methodology transitioned from single-molecule baseline estimates to complex multi-ligand simulations, enabling simultaneous docking of identical or diverse small molecules within the extended active site. To ensure exhaustive sampling of the potential energy surface, we performed configurational sampling with at least 10000 accepted configurations for each investigated system.[2] The resulting dataset was further processed using parallelized geometry optimizations and binding energy calculations to ensure accuracy and computational efficiency. Our previous findings reveal that the hBChE active site supports stable multi-ligand occupancy, with specific configurations demonstrating clear synergistic binding affinities that exceed those of single-ligand interactions.[3,4] This cooperative binding behavior suggests that the active site can accommodate multiple fragments in a manner that significantly enhances overall stability. These results provide a critical structural blueprint for the rational design and synthesis of larger, fragment-linked inhibitors characterized by increased potency and specificity, offering a promising pathway toward the development of more effective therapeutic agents for Alzheimer's disease.

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ALICE & BOB MEET ON ZIGZAG POLYHEXES

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Toroidal and zigzag Klein-bottle (KB) fullerenes share a peculiar topological symmetry whose existence has been recently proposed [1]. This symmetry holds for certain lattice size ratio. Here the main properties of the symmetry are presented as a comparison of Alice / Bob polyhexes, whose topological distance-based invariants gradually *overlap* from just two lines of vertices with the same transmission value till the complete match valid for all graph nodes when the specific threshold size has reached, triggering the transition into the Tori-KB symmetry region. Some extension of current investigation are proposed.

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TUNING DOMAIN-BASED CHARGE TRANSFER IN ORGANIC DYES: IMPACT OF HETEROATOM DOPING ON THE π-LINKER OF CARBAZOLE-BASED SYSTEMS

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This work presents an innovative computational study of domain-based charge transfer[1] that leverages the localized orbitals of pair coupled cluster doubles (pCCD). This method (EOM-pCCD+S)[2] enables both directional monitoring and quantitative assessment of charge transfer among donor (D), bridge (B), and acceptor (A) moieties. We applied this approach to a series of newly designed carbazole-based prototypical organic dyes, doping the bridge at positions 1, 2, and 3 with nitrogen, oxygen, and sulfur atoms to generate mono-, di-, and tri-doped variants. Our results demonstrate a clear and progressive enhancement in charge transfer as the degree of nitrogen or oxygen doping increases from mono- to di- to tri-doped systems. For mono-doped dyes, the highest forward charge transfer from donor to bridge to acceptor (D → B → A) occurs when a heteroatom (N or O) is placed in the terminal ring of the bridge, closer to the acceptor. In di-doped dyes, the largest forward charge transfer is observed when heteroatoms occupy both terminal positions, with one atom (N or S) adjacent to the donor and the other (N) near the acceptor. Nitrogen-doped systems consistently outperform their oxygen and sulfur counterparts. Among all variants, the organic dye doped with three nitrogen atoms at the bridge exhibits the most efficient and highest directional donor-to-acceptor charge transfer (42.6%), making it the most promising candidate for potential applications in dye-sensitized solar cells.

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QUANTUM MECHANICAL ANALYSIS OF THE MEASLES VIRUS FUSION PROTEIN–INHIBITOR COMPLEX

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The measles virus is a highly contagious pathogen for which no effective antiviral therapy is currently available, and treatment remains largely symptomatic despite widespread vaccination. Viral infection is initiated when the hemagglutinin (H) protein binds to the host cell receptor, thereby triggering membrane fusion mediated by the fusion (F) protein.

Recent structural studies[1] have reported the complex structure of the F protein bound to the fusion inhibitor AS-48, enabling molecular-level discussion of its inhibitory mechanism (Figure 1).

Here, we applied the fragment molecular orbital (FMO) method[2,3] to the F protein–AS-48 complex and analyzed interfragment interaction energies (IFIEs). AS-48 was shown to stabilize the prefusion conformation by bridging spatially separated residues, thereby inhibiting membrane fusion. Key residues involved in binding were identified, and their interaction energies with AS-48 were quantitatively evaluated. Furthermore, to advance understanding of the molecular recognition mechanism, derivatives of AS-48 were virtually constructed, and their interactions with the F protein were also analyzed. These physicochemical parameters provide insight into the molecular recognition mechanism and may guide the design of novel inhibitors.

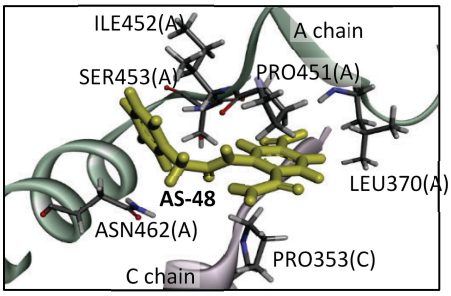

Figure 1. Position of AS-48 (yellow) and the surrounding amino acid residues. (PDB ID: 5YZC)

Table 1. IFIEs of Amino acid residues interacting with AS-48.

Residue (Chain)	IFIE (kcal/mol)
LEU370 (A)	–6.77
PRO451 (A)	–3.02
ILE452 (A)	–23.95
SER453 (A)	–5.22
LEU454 (A)	–4.16
ASN462 (A)	–8.89
THR461 (B)	–4.74
GLU471 (B)	–4.95
PRO350 (C)	–3.67
SER352 (C)	–4.30
PRO353(C)	–6.85

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ANALYTIC GRADIENTS AND GEOMETRY OPTIMIZATION FOR ORBITAL-OPTIMIZED PAIR COUPLED CLUSTER DOUBLES

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We introduce a reusable geometry-optimization engine in PyBEST for analytic, gradient-driven molecular structure optimization, with particular emphasis on orbital-optimized pair coupled-cluster doubles (OOpCCD/AP1roG).[1] The engine interfaces PyBEST with the geomeTRIC optimizer, combining analytic electronic-structure gradients from PyBEST with the translation–rotation–internal coordinate (TRIC) framework and robust convergence machinery.[2] Specifically, we present the first implementation of analytic OOpCCD nuclear gradients within a Lagrangian formalism.[3] The approach is generally applicable to seniority-zero wavefunctions with orbital optimization and response one- and two-particle reduced density matrices. Owing to the seniority-zero structure of pCCD and orbital stationarity, the gradient equations are compact, reduce the storage of the two-particle reduced density matrix, and avoid finite-difference differentiation of wavefunction parameters. Validation on representative closed-shell systems shows that the PyBEST–geomeTRIC workflow converges robustly and reproduces reference equilibrium geometries and energies within tight tolerances.[4] OOpCCD structural parameters deviate by about 0.02 Å from CCSD(F12c)(T*) and about 0.01 Å from MP2 reference bond lengths, while bond-angle deviations are generally below 1°.

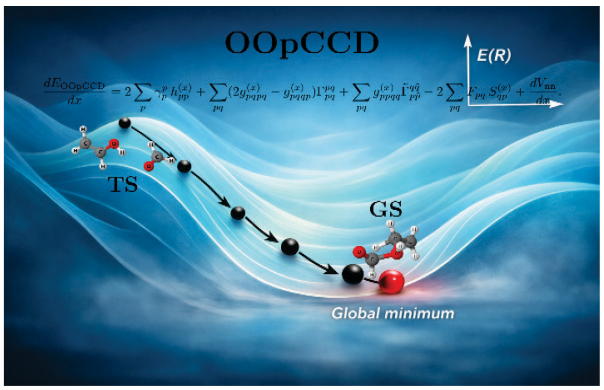

Figure 1. Schematic overview of OOpCCD-based geometry optimization.

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RELIABLE IONIZATION POTENTIALS FROM KOOPMANS'-BASED FRAMEWORK WITH PCCD WAVEFUNCTIONS

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Accurate prediction of ionization potentials (IPs) and orbital energies is essential for understanding charge-transfer processes in organic electronic materials, yet remains challenging due to the treatment of electron correlation. In this work, we develop efficient computational strategies within the pair Coupled Cluster Doubles (pCCD) framework and its orbital-optimized variant (oo-pCCD) to obtain reliable IPs at reduced computational cost. We formulate Koopmans'-type approaches [1] based on similarity-transformed pCCD Hamiltonians, introducing correlation-corrected expressions for orbital energies. These models are further extended through the Extended Koopmans' Theorem [2], where IPs are obtained from reduced density matrices derived from pCCD wavefunctions. Additionally, ionization potential equation-of-motion pCCD (IP-EOM-pCCD) methods are employed as reference data for IPs. Benchmark calculations for atoms and organic acceptor molecules demonstrate that pCCD-based Koopmans' and Extended Koopmans' Theorem [3] approaches significantly improve IP predictions over standard Hartree–Fock Koopmans' theorem, while maintaining favorable computational scaling. The use of pCCD natural orbitals enhances numerical stability and reduces sensitivity to basis-set effects. Our results show that pCCD-based methods available in the PyBEST software package [4], offer a scalable and accurate alternative to conventional wavefunction techniques.

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