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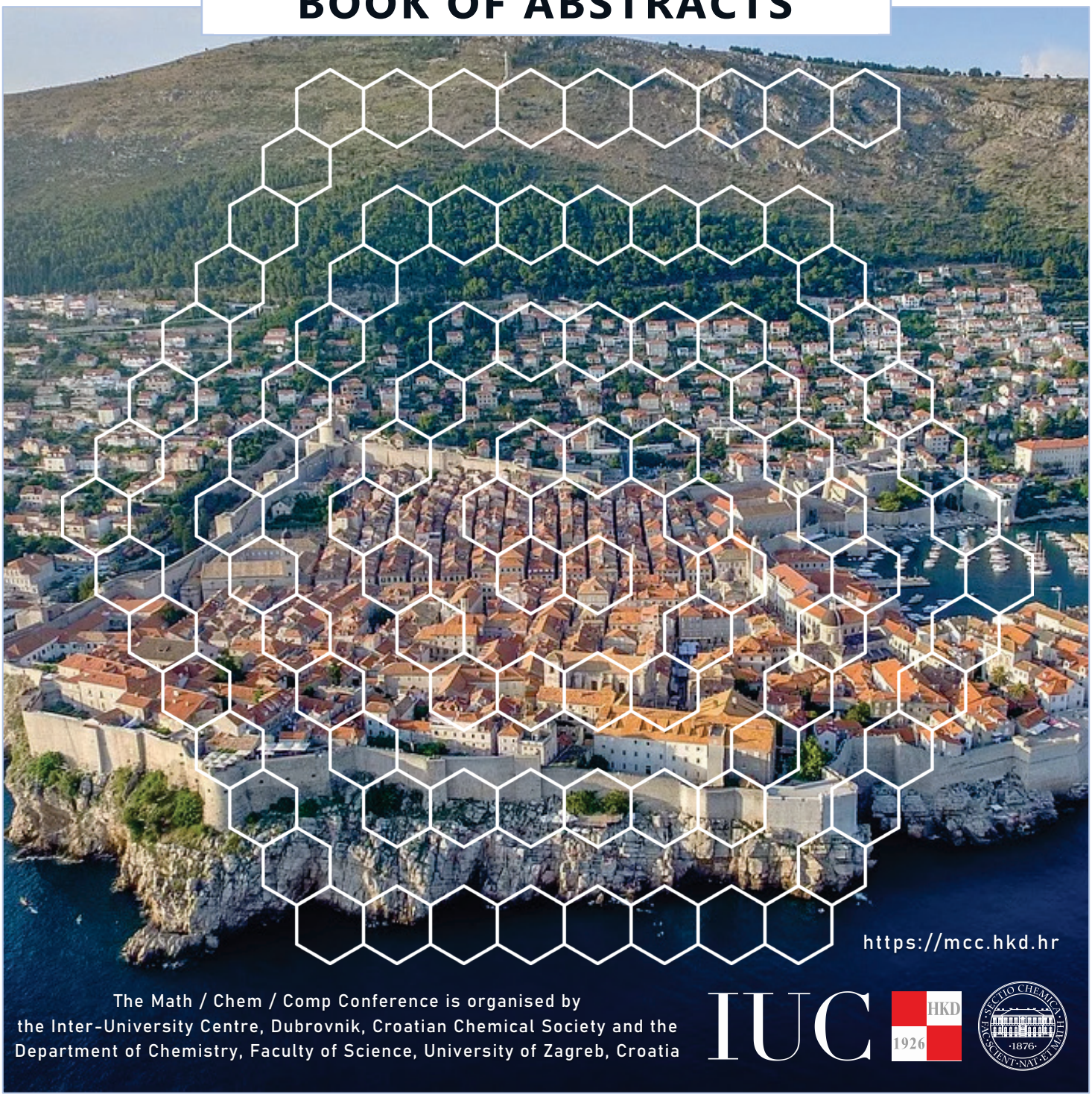
Math/Chem/Comp 2024 – 35th MC² Conference

Inter University Centre Dubrovnik, 3 – 7 June 2024

BOOK OF ABSTRACTS



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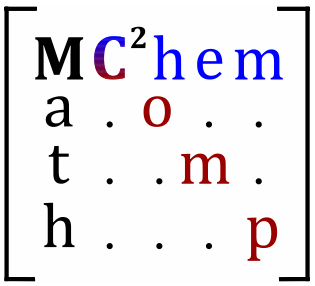

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IMPRESSUM

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Don Frana Bulića 4
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https://iuc.hr/
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The 35th International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences: Mathematics, Chemistry, Computing (Math/Chem/Comp, MC^2-35)

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^2-35 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
5. **Special section: Complexity**
6. **Special section: Few-electron systems**

The conference program will include invited lectures, contributed oral presentations, and posters. Moreover, we will offer a **Workshop**: "Special topics in the theory of angular momentum" which will be held by **Henryk Witek**, Professor of Chemistry, National Yang Ming Chiao Tung University, Taiwan.

Proceedings

The papers presented at the MC^2-35 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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MONDAY, JUNE 3	
8:00 – 9:00	**REGISTRATION**
9:00 – 9:20	**CONFERENCE OPENING (Hrvoj Vančik / Jerzy Cioslowski)**
CHAIR: Jerzy Cioslowski	
9:20 – 10:00	**Michael Melgaard:** *Density Functional Theory With Magnetic Fields: A Spectral Approximation Scheme*
10:00 – 10:30	**Andreas Savin:** *A Modified Expression for the Hamiltonian Expectation Value Exploiting the Short-Range Behavior of the Wave Function*
10:30 – 11:10	**Tomasz A. Wesolowski:** *The Failure of Gradient Expansion Approximation in Case of the Bi-Functional for Non-Additive Kinetic Potential*
11:10 – 11:30	**COFFEE BREAK**
11:30 – 12:00	**Stephen G. Dale:** *Variational Density Functional Theory Using the Jax Deep-Learning Differentiable Framework*
12:00 – 12:40	**Jacek Karwowski:** *Reflections on a Certain Density Functional: Is This a Warning or Maybe Ariadne's Thread?*
12:40 – 13:10	**Artur Ishkhanyan:** *Generalisation of the Second Demkov-Kunike Level-Crossing Quantum Two-State Model*
13:10 – 15:00	**LUNCH BREAK**
CHAIR: Andreas Savin	
15:00 – 15:30	**Katharina Boguslawski:** *Toward Alternative Wave Function Ansätze for Organic Electronics*
15:30 – 16:30	**John M. Herbert:** *High-Fidelity Fragmentation Methods in Quantum Chemistry*
16:30 – 16:50	**COFFEE BREAK**
16:50 – 17:30	**Miquel Solà:** *NICS and Ring Currents - An Exploration of Failures and Limitations*
17:30 – 18:00	**Valera Veryazov:** *Electronic Structure of Ionic Crystals with Ab Initio Methods*
18:00 – 18:40	**Branimir Bertoša:** *Allosteric Mechanisms of Selected Manganese Metallosensors*

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

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

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

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

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

LECTURES

DENSITY FUNCTIONAL THEORY WITH MAGNETIC FIELDS: A SPECTRAL APPROXIMATION SCHEME

Michael Melgaard[a] and Ville J. J. Syrjänen[b]

[a] School of Mathematical and Physical Sciences, University of Sussex, United Kingdom.
m.melgaard@sussex.ac.uk

[b] Faculty of Engineering, Kyoto University of Advanced Science, Japan.
ville.syrjaenen@kuas.ac.jp

We provide a mathematical justification of a spectral approximation scheme known as spectral binning for the Kohn-Sham spin density-functional theory in the presence of an external (nonuniform) magnetic field and a collinear exchange-correlation energy term. We use an extended density-only formulation for modeling the magnetic system. No current densities enter the description in this formulation, but the particle density is split into different spin components. By restricting the exchange-correlation energy functional to be of a collinear LSDA form, we prove a series of results which enable us to mathematically justify the spectral binning scheme using the method of Gamma-convergence, in conjunction with auxiliary steps involving recasting the electrostatic potentials, justifying the spectral approximation by making a spectral decomposition of the Hamiltonian and linearizing the latter.

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A MODIFIED EXPRESSION FOR THE HAMILTONIAN EXPECTATION VALUE EXPLOITING THE SHORT-RANGE BEHAVIOR OF THE WAVE FUNCTION

Jacek Karwowski, Anthony Scemama, and Andreas Savin

Laboratoire de Chimie Theorique, CNRS and Sorbonne University, 4, place Jussieu, 75252 Paris, France
andreas.savin@lct.jussieu.fr

Abstract: The expectation value of the Hamiltonian using a model wave function is widely used to estimate the eigenvalues of electronic Hamiltonians. We explore here a modified formula for models based on long-range interaction. It scales differently the singlet and triplet component of the repulsion between electrons not present in the model (its short-range part). The scaling factors depend uniquely on the parameter used in defining the model interaction, and are constructed using only exact properties. We show results for the ground states and low-lying excited states of Harmonium with two to six electrons. We obtain important improvements for the estimation of the exact energy, not only over the model energy, but also over the expectation value of the Hamiltonian. An asymptotic lower bound can also be constructed.

THE FAILURE OF GRADIENT EXPANSION APPROXIMATION IN CASE OF THE BI-FUNCTIONAL FOR NON-ADDITIVE KINETIC POTENTIAL

Tomasz A. Wesolowski

Dépt. Chim. Phys., Université de Genève, 30 quai Ernest-Ansermet, 1211 Genève, Switzerland
tomasz.wesolowski@unige.ch

The non-additive kinetic energy bi-functional ($T_s^{nad}[\rho_A,\rho_B] \equiv T_s[\rho_A+\rho_B]-T_s[\rho_A]-T_s[\rho_B]$) and its partial functional derivative wrt. ρ_A ($v_s^{nad}[\rho_A,\rho_B](\mathbf{r})$) are key elements in various embedding methods based on Frozen-Density Embedding Theory (FDET) [1]. The potential $v_s^{nad}[\rho_A,\rho_B](\mathbf{r})$ is one of the component of the total FDDT embedding potential used in the FDET eigenvalue equation. In the first part, we overview our works demonstrating that the failure of the "top-down" strategy to approximate $v_s^{nad}[\rho_A,\rho_B](\mathbf{r})$. Improvement of accuracy of a given approximation for $T_s[\rho]$ doeas not improve the accuracy of the potential $v_s^{nad}[\rho_A,\rho_B](\mathbf{r})$ [2]. In the main part, we overview our works on approximating $v_s^{nad}[\rho_A,\rho_B](\mathbf{r})$ based on imposing certain conditions directly on $v_s^{nad}[\rho_A,\rho_B](\mathbf{r})$ [2]. The considered conditions reflect the exact physical or mathematical properties of the FDET embedding potential.

REFERENCES

[1] The exact FDET relations between the embedding potential and the Hohenberg-Kohn density functional are given in [T.A. Wesolowski, *Phys. Rev. A.* **77** (2008) 012504] and in [T.A. Wesolowski, *J. Chem. Theor. & Comput.* **16** (2022) 6880-6885].

[2] E. Polak, C.E. Gonzalez-Espinoza, M.J. Gander, and T.A. Wesolowski. *J. Chem. Phys.* **156** (2022) 044103 and the references there.

VARIATIONAL DENSITY FUNCTIONAL THEORY USING THE JAX DEEP-LEARNING DIFFERENTIABLE FRAMEWORK

Stephen G. Dale[a,*], Tianbo Li[b], Zekun Shi[b,c], Giovanni Vignale[a], A. H. Castro Neto[b,d], Kostya S. Novoselov[a]

[a] Institute for Functional Intelligent Materials, National University of Singapore, Block S9, Level 9, 4 Science Drive 2, Singapore 117544
sdale@nus.edu.sg

[b] Sea AL Labs, 1 Fusionopolis Place, #17-10, Galaxis, Singapore 138522

[c] School of Computing, National University of Singapore, COM1, 13 Computing Dr, Singapore, 117417

[d] Centre for Advanced 2D Materials, National University of Singapore, 6 Science Drive 2, Singapore 117546

Variational density functional theory (VDFT) is a state-of the-art method for computing the electronic structure of materials in which the traditional self-consistent field (SCF) approach (i.e. solving the Kohn-Sham equation to self-consistency) is converted to a direct-gradient-descent minimization of the total energy with respect to one-electron orbitals and an occupation function, subject to orthogonality constraints. The main advantages of this approach are:

1. the optimization can be executed within a deep-learning differentiable framework.
2. convergence properties are expected to improve. The new optimization methods available through deep-learning will not be susceptible to the same instability present in SCF methods, and will be resistant to becoming stuck in saddle-points as in standard gradient-descent methods.
3. Kohn-Sham eigenvalues and eigenfunctions can be obtained by a *single* diagonalization of the Kohn-Sham Hamiltonian matrix.

At the heart of our method is a novel reparameterization of the orthogonality constraint by QR decomposition.[1] Our programs are written using Google's JAX deep-learning framework and are designed to be end-to-end differentiable to provide additional tools that are essential for discovery and design of advanced materials. Ultimately any available input variable can be targeted by the direct-gradient-descent optimization function, enabling; alchemical analysis by making nuclear charge a variable; on-the-fly adjustment of density functional parameters; and incorporation of neural networks to train a wide range of solutions.

Experiments are carried out to demonstrate the advantages of our approach in terms of stability. We deliberately choose chemical systems that are known to be challenging for SCF methods and show that our method can reliably converge these. We construct a gradient-only based approach to geometry convergence that can simultaneously converge the electronic and the atomic structure. We will show that we can reliably predict the band structure and the potential energy surfaces of crystalline materials.[2] Finally, we discuss some of the cutting-edge applications we are actively working towards.

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[2] Tianbo Li, Stephen Gregory Dale, Zekun Shi, Jingshu Li, Giovanni Vignale, A. H. Castro Neto, Kostya S. Novoselov, OpenReview, (2023).

REFLECTIONS ON A CERTAIN DENSITY FUNCTIONAL: IS THIS A WARNING OR MAYBE ARIADNE'S THREAD?

Jacek Karwowski

Instytut Fizyki, Uniwersytet Mikołaja Kopernika, ul. Grudziądzka 5, 87-100 Toruń, Poland
jka@umk.pl

Some exotic properties of exact density functionals derived from the multicomponent Dirac-Coulomb model and from its non-relativistic limit are discussed. In particular:

1. For the hydrogen-like atoms, the variational minima of both functionals are equal to the exact energies, as expected. But, it appears that these minima can be reached by an infinite set of densities [1].

2. For all helium-like atoms, the ground state energies, with the accuracy up to 1 milihartree, have been obtained using a simple two-parameter density. One of the parameters has been determined variationally, and the second one derived from the asymptotic properties of the averaged one-electron density of helium-like atoms [2].

The results can be considered a counterexample to the expectation that the better the energy value, the more correct the density. On the other hand, the surprisingly good results for two-electron atoms, in both relativistic and non-relativistic regimes, indicate that the properties this functional deserve detailed examination.

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[2] E. Z. Liverts and R. Krivec, *J. Math. Phys.* **61** (2020) 032105.

GENERALISATION OF THE SECOND DEMKOV-KUNIKE LEVEL-CROSSING QUANTUM TWO-STATE MODEL

Artur Ishkhanyan

Institute for Physical Research of Armenian NAS, Ashtarak, 0203 Armenia, aishkhanyan@gmail.com

The two Demkov-Kunike level-crossing two-state models [0] are prominent field-configurations used in the past to explore various aspects of non-adiabatic transitions in basic two-state quantum systems in both linear and nonlinear processes [0-0]. These models are members of the four well-known classical ordinary-hypergeometric classes of exactly solvable two-state models studied by several authors [0,7].

Recently, it has been shown that these ordinary-hypergeometric families can be significantly generalized if the solutions of the two-state problem are considered in terms of the five advanced Heun functions [8]. In particular, when the general Heun function is applied, there are 11 independent infinite classes (out of a total of 35 [9]) of exactly solvable general-Heun classes of models. The classes offer a rich variety of field configurations with various useful physical properties, in particular, constant-amplitude models of single, double, or multiple crossings of the frequency resonance (generally, asymmetric in time) or glancing the resonance.

In the present communication, we employ a solution of the general Heun equation in terms of the Clausen generalized hypergeometric functions to construct a novel two-state model that is exactly solvable in terms of the Gauss ordinary hypergeometric functions. The model describes a level-crossing process in a two-state quantum system subjected to excitation by a constant-amplitude laser field with a detuning that always varies asymmetrically with time. Since the amplitude is constant and the detuning varies within a limited interval, this excitation model can be perceived as an asymmetric generalization of the second Demkov-Kunike model [0].

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TOWARD ALTERNATIVE WAVE FUNCTION ANSÄTZE FOR ORGANIC ELECTRONICS

Katharina Boguslawski

[a] Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Grudziądzka 5, 87-100 Toruń, Poland
k.boguslawski@fizyka.umk.pl

Quantum-mechanical modeling can assist experimental studies in efficiently devising novel compounds with desired properties. However, the computational models are also difficult primarily because conventional highly-accurate quantum chemistry approaches are technically limited to small—and to some extent rather simplified— model compounds and demand user control on an expert level. Thus, innovative new electronic structure tools are desirable that do not suffer from the technical bottlenecks and shortcomings of conventional machineries and that open up new frontiers for ab initio computational chemistry. To this end, we will discuss alternative wave-function-based approaches that represent computationally inexpensive, robust, and black-box-like electronic structure methods. Specifically, we will focus on electron-pair theories, where two-electron functions are the fundamental building blocks of the electronic wave function, and how they can be extended to obtain a balanced description of static/nondynamic and dynamic correlation. Furthermore, we will scrutinize their performance to describe the electronic structures of both closed- and open-shell molecules in electronic ground and excited states.

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HIGH-FIDELITY FRAGMENTATION METHODS IN QUANTUM CHEMISTRY

John M. Herbert

Department of Chemistry & Biochemistry, The Ohio State University, Columbus, Ohio USA
herbert@chemistry.ohio-state.edu

Fragmentation methods offer the promise of defeating the nonlinear scaling of ab initio electronic structure theory and thus extending computational quantum chemistry to sizable molecular systems, using what amounts to a multiscale treatment of the electron correlation problem.[1] Too often, however, accuracy considerations have been secondary to demonstrations of scalability, with little consideration for what types of computational problems genuinely require what remains a relatively expensive approach, at least in comparison to QM/MM methods. My group has pursued high-fidelity fragment-based approximations that target sub-kcal/mol accuracy with respect to a full-system calculation at a well-defined level of theory.[2–4] We insist on methods that are stable and robust at arbitrary levels of electronic structure theory, including large basis sets containing diffse functions, and for arbitrary protonation states in the case of enzymatic applications.[5] Such methods can reliably be used to extrapolate to both the ab initio limit[6,7] as well as the system-size limit. This is tractable by means of multilayered approximations and a novel energy-based screening approach,[8] based on a bottom-up graph theory algorithm.[9] This is essential in order to surmount a sizable combinatorial bottleneck in large systems, where the number of requisite subsystem calculations may exceed 10^6. I will describe the implementation of these methods within a new, open-source Python package called FRAGME∩T,[10] developed in my group and used to tackle ab initio applications of unprecedented size. These include converged thermochemical calculations for enzyme-catalyzed reactions (using enzyme models with 600+ atoms),[5] converged ligand-protein binding energies using even larger model systems, and converged many-body expansions for water clusters and ion-water clusters including up to eight-body terms.[9]

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NICS AND RING CURRENTS - AN EXPLORATION OF FAILURES AND LIMITATIONS

Miquel Solà

Institut de Química Computacional and Departament de Química, Universitat de Girona, C/ Maria Aurèlia Capmany 69, 17003 Girona, Catalonia, Spain
miquel.sola@udg.edu

Among the different indicators of aromaticity, the magnetic-based descriptors hold a prominent place [1]. A large number of studies rely only on magnetic indicators of aromaticity to prove whether a given system is aromatic, non-aromatic or antiaromatic. Although in many cases, these magnetic indicators of aromaticity provide a good description of the aromaticity of the systems studied, there are examples of failures of these indicators to correctly account for their aromaticity. In this lecture, we will discuss some examples of these failures that we and others have found in the investigation on the aromaticity phenomenon [2–7]. Our final conclusion would be that to characterize aromaticity one has to used several indices based on the different properties aromatic compounds have.

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ELECTRONIC STRUCTURE OF IONIC CRYSTALS WITH *AB INITIO* METHODS

Valera Veryazov

Computational Chemistry, Lund University, Lund 22100, Sweden.
valera.veryazov@teokem.lu.se

Multiconfigurational theory [1] is known for its accuracy and reliability, yet the high cost of calculations typically restricts its application range. Traditionally, this theory is used for small molecules containing only a few atoms. However, recent advances in the theory, coupled with complementary methods such as embedding [2], compact basis sets [3] and efficient computational codes [4], enable its application to clusters. These clusters can model the electronic structure of ideal crystals, surfaces, and crystals with point defects.

The lecture showcases several examples of applying multiconfigurational theory to electronic structure calculations across various materials, ranging from simple metal oxides to crystals with complex structures such as mixed oxides, garnets, and perovskites. Special attention is devoted to issues concerning ions mobility and electronic spectroscopy [5].

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ALLOSTERIC MECHANISMS OF SELECTED MANGANESE METALLOSENSORS

Branimir Bertoša

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10000 Zagreb, Croatia
bbertosa@chem.pmf.hr

Since manganese ions (Mn^{2+}) are necessary for some of essential cellular processes in bacteria, such as DNA replication and resistance to oxidative stress, manganese homeostasis is also essential for bacteria.[1,2] Homeostasis of Mn^{2+} ions in bacteria cells is regulated by managanese metallosensors – transcriptional factors that regulate transcription of proteins involved in transport and storage of Mn^{2+} ions in cell. Allosteric mechanism(s) of manganese metralosensors from selected bacteria were studied computationally and experimentally. Computational methods consisted primarily of molecular dynamics (MD) simulations. Starting from available crystal structures, different systems with and without Mn^{2+} ions in the binding sites were generated *in silico* and prepared for all-atom MD simulations using explicit solvent model. Parametrisation of interactions between Mn^{2+} ions and amino acid residues of the binding sites were achieved using quantum mechanics (QM) calculations. Computational results provided insight into molecular basis of differences in structural and dynamical properties of selected manganese metallosensors regarding the presence or absence of Mn^{2+} ions in the binding sites. Based on these results, experimental investigation was planned and conducted in order to validate allosteric model proposed according to computational results. Several different experimental methods, such as microcalorimetry (ICT and DSC), circular dichroism (CD) spectroscopy, and electron paramagnetic resonance (EPR) were used. Sinergy of computational and experimental results enabled reliable conclusions about the allosteric mechanisms through which Mn^{2+} ions increase DNA binding affinities of selected manganese metallosensors.[3-5] Results showed that in some cases significant conformational changes of a protein were induced by Mn^{2+} binding.

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SYMMETRY EQUIINCIDENCE OF NATURAL ORBITALS

Jerzy Cioslowski

Institute of Physics, University of Szczecin, Wielkopolska 15, 70-451 Szczecin, Poland
jerzy.cioslowski@usz.edu.pl

The symmetry equiincidence principle quantifies the apportionment of the natural orbitals (NOs), ordered according to their nonascending occupation numbers, among the irreducible representations (irreps) of the point group pertaining to the underlying on-top two-electron density. This principle, which is rigorously proven for the resolvable C_s, C_{2v}, C_{3v}, C_{4v}, C_{6v}, D_{2h}, D_{3h}, D_{4h}, D_{6h}, and O_h point groups, states that the symmetry incidences, i.e. the asymptotic probabilities with which the NOs belonging to different irreps occur, are proportional to the squares of irreps' dimensions. Since its proof hinges upon a sufficient number of planes of symmetry among the elements of a given point group, it yields only linear combinations of the symmetry incidences for the quasiresolvable groups with too few such planes and fails for the unresolvable C_1, C_i, C_n, D_n, S_{2n}, T, O, and I groups whose nontrivial elements comprise only symmetry axes and/or the center of inversion.

SEPARATION OF ROTATIONAL DEGREES OF FREEDOM IN QUANTUM THREE-BODY SYSTEM

Anjan Sadhukhan,[a] Grzegorz Pestka,[b] and Henryk A. Witek[c]

[a] Department of Applied Chemistry, National Yang Ming Chiao Tung University, 1001 University Road, Hsinchu, 300 Taiwan, anjanphy21@gmail.com

[b] Faculty of Engineering and Technology, State Academy of Applied Sciences in Włocławek, ul. 3 Maja 17, 87-800 Włocławek, Poland, gp@fizyka.umk.pl

[c] Department of Applied Chemistry, National Yang Ming Chiao Tung University, 1001 University Road, Hsinchu, 300 Taiwan, hwitek@nycu.edu.tw

Separation of variables in the case of the Schrödinger equation (SE) for a non-relativistic quantum three-body system (QTBS) has been an interesting topic of research for a long time. In principle, due to the rotational and translational invariance of the system, the nine-dimensional SE can be reduced to a system of three-dimensional partial differential equations (PDEs), referred in the following as the reduced radial SE (RRSE). The reduction of the SE to a set of three-dimensional PDEs through the separation of the angular variables is most challenging and tricky job. Breit's seminal work [1] reduced the SE to a set of two PDEs for P^o states, in terms of the internal coordinates proposed by Hylleraas [2]. Further extension of this problem to arbitrary angular momentum was revisited many times by different researchers [3–9], contributing to better conceptual understanding of the whole problem.

We report a novel straightforward technique to derive the RRSE of the non-relativistic QTBS in the basis of solid bipolar spherical harmonics (BSH) for arbitrary angular momentum and parity states. The resulting RRSE is identical to the equation reported previously in the literature [6]. We propose an ansatz regarding the correspondence of BSH and Wigner-D functions, which has not been reported earlier to the best of our knowledge. This relation simplifies angular matrix element evaluation compared to prior methods [5,10]. The validity of the reported relations has been confirmed by estimating energy eigenvalues for selected low-lying angular momentum states of the helium atom.

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BOUND STATE STABILITY IN FEW PARTICLE SYSTEMS USING NUMERICAL METHODS

Hazel Cox

Department of Chemistry, University of Sussex, Brighton, BN1 9QJ, UK
h.cox@sussex.ac.uk

As high-precision experiments become more sophisticated, and systems probed become more complex, it's important to ensure theory remains an essential tool for interpreting and predicting chemical systems and phenomena. Three-body Coulomb systems are the simplest that capture the effects of electron correlation and nuclear motion and are therefore of interest for atomic and molecular theory, for systems containing various elementary particles such as muons and positrons, and as a testbed for new method developments.

High-accuracy, non-relativistic, quantum chemical calculations of the energy levels and wavefunctions of three-particle systems are calculated using a fast and efficient series solution method in a triple orthogonal Laguerre basis [1] and using a numerical tensor method with either a finite-element approach in combination with a low rank tensor decomposition [2] or more recently, using a low rank tensor decomposition with a triple orthogonal Laguerre basis.

The series solution method [1], is adapted to calculate, in a single variational calculation, the critical mass or charge for bound state stability, and a Hartree-Fock implementation. The effects of nuclear motion [3], and high-accuracy benchmark electron correlation data [4], will be presented. Exploring the correlated motion of electrons at low nuclear charge just prior to electron-detachment and attempting to capture this behaviour in future theoretical method developments, such as correlation functionals [5,6], is an important step forward. It will also be shown that by using a low-rank tensor decomposition a significant reduction in computational complexity is achieved without compromising the accuracy.

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ROVIBRATIONAL ENERGY LEVELS OF THE HYDROGEN MOLECULE AND ITS ISOTOPOLOGUES FROM RELATIVISTIC NONADIABATIC CALCULATIONS

Jacek Komasa,[a] and Krzysztof Pachucki[b]

[a] Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland; komasa@man.poznan.pl

[b] Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland; k.pachucki@uw.edu.pl

The energy of a molecular rovibrational level is theoretically derived from several components, including nonrelativistic, relativistic, quantum electrodynamics, and more. When it comes to a light molecule such as hydrogen or its isotopologue, the nonrelativistic quantum electrodynamics (NRQED) can accurately describe this energy using an expansion in powers of the fine structure constant. The component that is least accurate in this expansion is limiting the accuracy of the total energy. Accurate predictions for hydrogen molecular levels require the treatment of electrons and nuclei on an equal footing. While nonrelativistic theory has been effectively formulated this way, calculations of relativistic and quantum electrodynamic effects with well-controlled numerical precision are much more challenging. In this communication, we report extending this nonadiabatic method to the relativistic correction term. The four-body nonadiabatic James-Coolidge wave function is applied to evaluate the expectation value of the Breit-Pauli Hamiltonian. The main obstacle encountered in this approach is the need for a whole class of new integrals resulting from combining relativistic operators with exponential basis functions. Such integrals have been successfully evaluated and new results of the relativistic correction will be reported. The convergence analysis indicates that the numerical uncertainty of this correction is of the order of 10^{-7} cm^{-1}. Similar to the nonrelativistic component, the uncertainty of the relativistic term is negligible enough to eliminate it from the overall uncertainty budget. An important aspect of the newly developed method is its capability of handling arbitrarily high rotational angular momentum without significant loss in accuracy. With the new relativistic results, the achieved accuracy is limited only by the uncertainty of the quantum electrodynamic effects.

Several recent experimental studies have revealed a minor discrepancy between the most precise theoretical and experimental data. This inconsistency offers an opportunity for further advancements in the field. It will be examined in light of new nonadiabatic relativistic calculations, providing insight into further improvements in the current theory.

ACCURATE CALCULATIONS OF FEW-ELECTRON SYSTEMS USING EXPLICITLY CORRELATED WAVE FUNCTIONS

Sergiy Bubin

Department of Physics, School of Sciences and Humanities, Nazarbayev University, Astana, Kazakhstan
sergiy.bubin@nu.edu.kz

Accurate calculations of few-particle systems, in particular small atoms, molecules, ions, and systems containing exotic particles, have always been a challenging task, especially if the goal of such calculations is to match or exceed the ever-increasing accuracy of spectroscopic measurements. The main obstacles arise from the treatment of the particle correlations, dealing with different energy and spatial scales for the motion of different particles, and accounting for relativistic and quantum electrodynamics effects. In this talk I will overview a conceptually simple approach for performing such calculations that is based on the variational method and expanding the wave functions in terms of basis functions that are explicitly dependent on all interparticle coordinates. This approach has been adopted in both chemistry and physics for calculating the ground, excited, and even scattering state properties of small quantum systems of various nature. I will outline the basic theoretical foundations, computational aspects, recent developments, and then will talk about applications that primarily focus on atomic systems: energy spectra, electron and positron affinities, oscillator strengths, fine structure. I will also touch on some aspects related to the non-Born-Oppenheimer quantum chemistry and the unified treatment of electrons and nuclei. Lastly, I will discuss some challenges that need to be overcome to extend the applicability of the existing ECG approaches to larger systems.

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FINE STRUCTURE OF THE DOUBLET P LEVELS OF FIVE-ELECTRON ATOMIC SYSTEMS CALCULATED WITHOUT THE BORN–OPPENHEIMER APPROXIMATION

Monika Stanke

Nicolaus Copernicus University in Toruń, ul. Gagarina 11, 87-100 Toruń, Poland
ms@umk.pl

Variational calculations for selected atomic systems with five electrons without the Born-Oppenheimer approximation will be presented. Particular attention will be paid to the fine structure of the energy levels. For some states, the present data are the first ever reported and can be useful in guiding future accurate spectroscopic measurements.

NONUNITARY PROJECTIVE TRANSCORRELATION INSPIRED BY THE F12 ANSATZ

Seiichiro L. Ten-no

Graduate School of System Informatics, Kobe University
tenno@garnet.kobe-u.ac.jp

Computing electronic structures in high accuracy is one of the most sig- nificant challenges in quantum chemistry and physics, while the exponential growth of the Hilbert space with the number of correlated electrons hinders the application of wavefunction theory to large molecules. There has been a re- cent resurgence in the interest of the transcorrelated (TC) method of Boys and Handy [1] primarily driven by two objectives: The first objective is to combine TC with approximate full configuration interaction (FCI) solvers. The second is to reduce the number of qubits in quantum simulations by downfolding the high energy contribution of the Hamiltonian.

Although the TC Hamiltonian is universal and terminating at 3-body in- teractions, the local nature of the Jastrow factor employed in TC obstruct to satisfy different cusp conditions for singlet and triplet pairs unlike F12 theory [2]. To mitigate this situation, we recently introduced an alternative nonunitary transcorrelation inspired by the F12 ansatz [3]. The effective Hamiltonian of this projective TC (pTC) theory features no spin-contamination with simultaneous satisfaction of the singlet and triplet cusp conditions. The basic ideas of pTC in comparison with F12 theory will be presented. We shall also discuss applica- tions of pTC to FCI solvers including the full coupled-cluster reduction (FCCR) that is a selected coupled-cluster method to reduce the excitation manifold and nonlinear operations with suitable screenings [4-5].

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DIMENSIONALITY REDUCTION TECHNIQUES FOR CHEMICAL REACTIONS: REACTION SPACE PROJECTOR AND NATURAL REACTION ORBITALS

Tetsuya Taketsugu

[a] Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, 060-0810 Japan
[b] Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, 001-0020 Japan, *take@sci.hokudai.ac.jp*

In quantum chemistry, the Intrinsic Reaction Coordinate (IRC) is crucial for understanding the fundamental processes of chemical reactions. Defined by the potential energy surface, the IRC has historically guided research into reaction mechanisms. Recent advances in automated reaction path search technologies now allow us to investigate these mechanisms through networks that include multiple reaction paths [1]. These networks facilitate a more detailed and interconnected discussion of reaction mechanisms. Each reaction path within the network is represented as a one-dimensional curve in a coordinate space of 3*N*-6 dimensions for a system of *N* atoms, forming a complex web of paths across a multidimensional space. Additionally, trajectories from ab initio molecular dynamics (AIMD) simulations provide dynamic pathways across this network. In this presentation, I will introduce the Reaction Space Projector (ReSPer) method [2-6], which employs dimension reduction techniques to analyze and project these networks and trajectories onto a unified, lower-dimensional space. I will also discuss the natural reaction orbital (NRO) method [7,8], which reveals the evolution of chemical bonds along a reaction path by mixing specific pairs of occupied and virtual NROs.

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EXPLORING THE CONNECTION BETWEEN ELECTRONIC AND POTENTIAL ENERGY THEORIES VIA REACTIVE ORBITAL ENERGY THEORY

Takao Tsuneda

[a] Department of Chemistry, Faculty of Science, Hokkaido University, Japan
[b] Graduate School of Science Technology and Innovation, Kobe University, Japan
takaotsuneda@sci.hokudai.ac.jp

Traditionally, electronic theories like the electronic theory of organic chemistry (ETOC) and the frontier orbital theory, have evolved independently from potential energy theories, which include reaction energy diagrams and molecular dynamics. No existing theory had previously linked these distinct frameworks. Reactive orbital energy theory (ROET) [1] is the first to delineate a connection between electronic and potential energy theories through the concept of orbital energy variance. ROET identifies reactive orbitals that exhibit the maximum orbital energy variance along the intrinsic reaction coordinate (IRC) on the potential energy surface, as the key drivers of chemical reactions. It has been established that the electron transfer between reactive orbitals in typical organic reactions closely aligns with the curly arrows of ETOC [2]. Recently, reactive intramolecular electrostatic force (RIEF) method integrates these frameworks further. This method employs the electrostatic force theory [3] within the framework of ROET to calculate how reactive orbitals affect molecular nuclei. It elucidates the impact of electron transfers on structural deformations during reactions. RIEF calculations along the IRC for various reactions have shown that for most reactions, these values significantly affect the structural deformations in the reaction direction. Considering that the direction of electron transfer from occupied to unoccupied reactive orbitals closely aligns with the curly arrows of ETOC, this result indicates that electronic motions extracted in electronic theory analyses are deeply involved in the formation of the IRC. Therefore, it can be interpreted that RIEF has clarified the relationship from electronic theory to potential energy theory.

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MANY-TO-ONE MAPPING IN ELECTRONIC STRUCTURE CALCULATIONS FOR FINITE AND INFINITE SYSTEMS

Dirk Andrae

[a] Institut für Chemie und Biochemie, Freie Universität Berlin, Arnimallee 22, D-14195 Berlin, Germany
dirk.andrae@fu-berlin.de

"There is nothing more practical than a good theory [...]" [1] – Problems of many-to-one mapping in electronic structure calculations are related to degeneracies, which are themselves a consequence of the symmetry of the system under study. If we consider, for example, a system where several electronic states share a common energy (eigen-)value, then reduction of symmetry (e.g. by distortion) likely leads to an at least partial removal of degeneracy. I will discuss, example by example, a few cases where degeneracy due to symmetry plays an important role in atomic and molecular electronic structure, in bond formation / dissociation processes and in molecule–surface interaction processes. Convenient handling of degeneracies still poses challenges to computational methods. But, in view of Ahlrichs' quote, the theory of symmetry turns out to be an exceptionally practical theory, even though it does not (and cannot) yield the complete solutions of electronic structure problems.

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DISCRETE SYMMETRIES IN SYSTEMS OF INDISTINGUISHABLE PARTICLES

Mira Diekmann and Robert Berger*

Fachbereich Chemie, Philipps-Universität Marburg, Germany
* robert.berger@uni-marburg.de

Discrete symmetries being related to parity (P), charge-conjugation (C) and time-reversal (T) or to permutational symmetries of indistinguishable particles play an important role for our understanding of the structure of matter and its fundamental interactions. The symmetrisation postulate, spin-statistics connection and generalised Pauli principle form the basis of the aufbau principle and the structure of the periodic table of the elements. In this talk, we will discuss the role and interplay between various discrete symmetries and outline possible searches for their violations in molecular systems.

ERROR MITIGATION STRATEGIES FOR NEAR-TERM QUANTUM ALGORITHMS

Rahul Maitra

Department of Chemistry, Indian Institute of Technology Bombay, Mumbai-400076, India
rmaitra@chem.iitb.ac.in

Quantum computers provide a lucrative platform for efficiently determining molecular energetics and associated properties. However, noise in current quantum hardware can cause significant errors, hindering quantum advantage. We propose to enhance the efficiency and accuracy of quantum algorithms by developing an optimal framework for introducing Zero Noise Extrapolation (ZNE) in near-term quantum algorithms. Our analysis evaluates the impact of various circuit folding strategies and extrapolation functions on the accuracy and efficiency of the associated energy convergence trajectory, and investigates the mechanisms behind the observed improvements. However, owing to the exponential overhead of such a technique, this approach is limited to only shallow quantum circuits. To overcome this, we have developed a graph neural network and regression-based hybrid architecture that explicitly considers the coupling map and associated gate errors of the quantum hardware. With the short coherence time that plagues NISQ devices, our model exploits the structure of various snippet sub-circuits adhering to the hardware connectivity, and is explicitly trained to learn the features quickly with shallow circuits. This training data is generated on the fly during ansatz construction using error-mitigated expectation values for shallower sub-circuits. Once trained, the model can predict accurate molecular energetics for arbitrarily deep ansatz circuits. This approach is expected to facilitate practical applications of quantum computing in fields related to molecular sciences, where it is essential to determine molecular energies accurately.

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ORBITAL-INTERACTION GRAPHS FOR SATURATED HYDROCARBONS

Douglas J. Klein

Foundational Sciences, Texas A&M University @ Galveston, Galveston, TX 77553-1675
kleind@tamug.edu

Orbital-interaction graphs for saturated hydrocarbons are described, in terms of "stellated" graphs (where each node of a stellated graph represents a bonding "hybrid" atomic orbital of the parent atom, which is a parent node of the correspondent unstellated molecular graph). Thence here studied are eigen-spectral features of stellated graphs (and associated molecules). The stellated-graph eigen-spectra are found to frequently split into equal numbers of + & – values for a wide range of parameters. Consequent Gershgorin-theorem-based bounds are obtained on the HOMO-LUMO gap between these + & – values.

CLUSTER ANALYSIS OF FULLERENE ISOMERS

Tomislav Došlić

[a] University of Zagreb Faculty of Civil Engineering, Kranjčevićeva 2, 10000 Zagreb, Croatia
doslic@grad.unizg.hr

It has been known for a long time that there are many more possible fullerene structures than there are observed stable fullerene isomers. Search for reliable indicators and predictors of stable isomers has been among the most important driving forces of ongoing research in fullerene graphs. A fullerene graph is a 3-regular, 3-connected, plane graph with only pentagonal and hexagonal faces. Its spectrum is the spectrum of its adjacency matrix. For a graph F_n on n vertices, its spectrum can be considered as a point in n-dimensional space. So, for a given number of atoms n, we compute spectra of all fullerene graphs on n vertices. The resulting n-dimensional point set serves as the vertex set of a geometric graph $G(n,d)$ obtained by connecting all points whose distance does not exceed a given positive parameter d. We analyze the properties of such geometric graphs, in particular, the increase of their number of edges and the emergence and evolution of connected clusters with increasing values of d.

EXPLORING DEGREE-BASED GRAPH INVARIANTS IN RANDOM GRAPHS AND CHAINS

Ali Iranmansh

Department of Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University,
P.O. Box 14115-137, Tehran, Iran
iranmanesh@modares.ac.ir

Random graphs and chains are fundamental constructs in graph theory, widely applicable in various fields such as physics, chemistry, networks, etc. Here, we present a comprehensive analysis of degree-based graph invariants in random graphs and chains. We integrate the findings from [1-4] to offer valuable insights into the expected values and variances of these invariants.

We begin by investigating degree-based invariants, such as the first and second Zagreb indices, and the forgotten index, in random graphs. Specifically, we examine two models: random graphs with a fixed number of vertices, and random bipartite graphs. For each model, we calculate the expected values of the Zagreb indices and the forgotten index, shedding light on their behavior and growth rates.

Expanding our exploration, we focus on inhomogeneous bipartite random graphs. By considering the first and second Zagreb indices and the forgotten topological index, we determine their expected values. Additionally, we establish upper and lower bounds for the probabilities of edge occurrences, enabling us to derive expected value bounds for these indices. These findings enhance our understanding of the properties of inhomogeneous bipartite random graphs.

Furthermore, we extend our analysis to random chains, specifically four types of random m-polygonal chains. Utilizing a comprehensive approach, we compute the expected values and variances of degree-based graph invariants. By incorporating previous results, we derive systematic formulas that provide a clear framework for evaluating these invariants.

Keywords: Random graphs, Random chains, Degree-based graph invariants, Zagreb indices, Forgotten index, Expected values, Variances.

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ON I_1-EMBEDDABILITY OF (CHEMICAL) HYPERGRAPHS

Gašper Domen Romih

Faculty of Mathematics and Physics, University of Ljubljana
gasper.romih@fmf.uni-lj.si

The Wiener index is probably one of the most studied graph indices in chemical graph theory. The cut method was used to calculate explicit formulas for Wiener index of several important chemical graphs. In this talk, we will demonstrate how (chemical) hypergraphs can be embedded into l_1 space and how the cut method can be used in this case. More specifically we will present some Clar structures and phenylenes as hypergraphs and then used developed method to compute their Wiener index.

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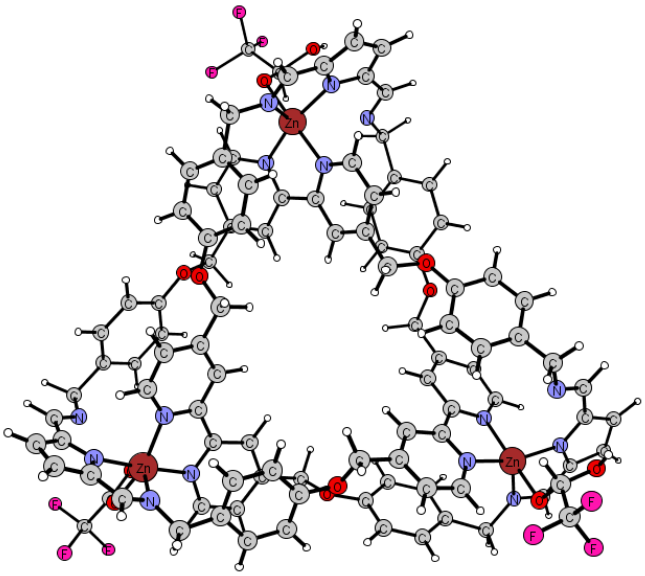
FAST COMPUTATIONAL METHODS TO STUDY LARGE AND COMPLEX MOLECULAR SYSTEMS

Bartosz Trzaskowski[a], J. P. Martinez[a], Bartosz Szyszko[b]

[a] Centre of New Technologies, University of Warsaw, Banacha 2C St., 02-097 Warszawa, Poland; b.trzaskowski@cent.uw.edu.pl

[b] Department of Chemistry, University of Wrocław, 14 F. Joliot-Curie St., 50-383 Wrocław, Poland; bartosz.szyszko@uwr.edu.pl

Quantum chemical computational methodologies may serve as predictive approaches to determine structures, topologies, cavity sizes, and associated molecular properties, both static and dynamic, for large molecular systems, such as organic cages, molecular knots and macrocyclic systems. This enables the guidance of synthetic researchers toward the identification and development of materials possessing targeted properties. Here we show the very fast and relatively accurate GFN2-xTB tight bonding approach and its applications to several large molecular systems. In particular, we use GFN2-xTB combined with DFT to study pyrrole cages encapsulating ion pairs and silver(I) clusters to form intricate supramolecular capsules [1,2]. We also show we that the time-dependent density functional theory UV–vis spectra may potentially serve as a diagnostic probe to characterize mixed-valence and geometrical configurations of silver clusters encapsulated into cryptands. In the second project, we show a that the diiminopyrrole coordination motif used in the design and construction of novel catenanes, trefoil knots, and Borromean rings rendered all new systems intrinsically flexible, as demonstrated by the combination of NMR spectroscopy, X-ray crystallography, and computational studies [3].



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A GPU-ACCELERATED IMPLEMENTATION OF THE DENSITY-FUNCTIONAL TIGHTBINDING METHOD

Cristopher Camacho

School of Chemistry, University of Costa Rica, 11501-2060, Costa Rica
cristopher.camacho@ucr.ac.cr

The requirement of accelerating calculations of complex chemical systems, e.g., molecular dynamics in the microsecond time scale, light harvesting processes carried out by biochemical complexes such as the photosystems associated to the photosynthesis, finds an answer in the use of graphical processing units (GPUs). Here, an implementation of the density-functional tight-binding (DFTB) method on single and multiple GPUs is presented.[1,2] The two major computational bottlenecks of DFTB ground-state calculations were addressed and the implementation was benchmarked to assess the speed-up.

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CORE-HOLE DELOCALIZATION EFFECTS IN COMPUTATIONAL X-RAY SPECTROSCOPY

Iulia Emilia Brumboiu,[a] Thomas Fransson[b]

[a] Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, 87-100 Toruń, Poland, iubr@umk.pl

[b] Department of Physics, AlbaNova University Center, Stockholm University, 109 61 Stockholm, Sweden, thomas.fransson@fysik.su.se

Here, I will provide an overview of different theoretical methods used to perform X-ray absorption, emission, and photoelectron spectroscopy calculations of organic molecules. A sometimes overlooked detail in these types of calculations is the use of an explicit core-hole to model orbital relaxation. For symmetric systems, the use of an explicit delocalized core-hole can produce large errors, while a localized core-hole is able to capture orbital relaxation well even at the Hatree-Fock or density functional theory levels. The source of this delocalization-induced relaxation error (DIRE) can be tracked down to an incomplete description of orbital relaxation by a delocalized core-hole. The issue can be ultimately alleviated by improving the treatment of electron correlation.

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PROTEIN INTERACTIONS OF DIPEPTIDYL PEPTIDASE III

Sanja Tomić,[a] Mihaela Matovina,[b] Sara Matić, Marko Tomin, Ana Tomašić Paić, Lucija Horvat, Lea Barbarić

[a] Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia, Sanja.Tomic@irb.hr
[b] Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia, Mihaela.Matovina@irb.hr

Within the last decade we intensively studied the zinc dependent exopeptidase dipeptidyl peptidase III (DPP III, EC 3.4.14.4), its enzymatic activity related to peptide hydrolysis,[1-4] and its 'moonlighting' activities accomplished through its interactions with other proteins.[5-7]

Herein, I will present results of our study of the interaction of DPP III with Kelch-like ECH-associated protein 1 (KEAP1) and SH2 domain-containing protein 3C (SH2D3C).

Utilizing synergy of theory and experiment we revealed that DPP III binding to KEAP1, a main sensor of the oxidative stress, is a two-step process involving endergonic translocation of the DPP III ETGE loop and exergonic binding to KEAP1.[5] We investigated how several DPP III mutations found in cancers affect affinity of DPP III for KEAP1 and the activity of KEAP1-NRF2 pathway.[6] NRF2 and its repressor KEAP1 are subjects of intensive research as attractive targets for prevention and treatment of the oxidative stress-related diseases, including cancer. Results of our research suggest that DPP III might also be a valuable target for therapeutic interventions in some cancers.

SH2D3C is a member of the family of adaptor proteins involved in the regulation of adhesion, migration, tissue organization and immune response. We showed that SH2D3C binds DPP III through its C-terminal domain, detected colocalization of the proteins in cells, computationally identified possible modes of binding and investigated how several DPP III cancer mutations located on protein interaction surface, influence stability of the DPP III – SH2D3C complex. The results of our study provide strong evidence for the validity of this interaction.[7]

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UNRAVELLING THE MOLECULAR MECHANISM OF ANTIMICROBIAL ACTIVITY OF TANNINS THROUGH JOINT EXPERIMENTAL AND COMPUTATIONAL MEANS

Urban Bren,* Sara Štumpf, Franjo Frešer, Miha Fermišek, Matja Zalar, and Gregor Hostnik

Faculty of Chemistry and Chemical Technology, University of Maribor, Smetanova 17, 2000 Maribor, Slovenia
* urban.bren@um.si

Depletion of essential metal ions from the growth medium through chelation represents a likely molecular mechanism behind the antimicrobial activity of tannins. Indeed, with an increase in the growth medium concentration, MIC values of all investigated tannins rose roughly linearly in the case of *E. Coli*, while their relative order remained unchanged, indicating that a direct interaction of tannins with growth medium nutrients represents the likely source of their antimicrobial activity.[1] Moreover, the generation times of *E. Coli* prolonged with increasing tannin concentration while the lag phase extended exponentially.[2] Similar findings were obtained also for *Staphylococcus Aureus*.[3] The UV/Vis spectra of gallic and ellagic acid pH dependence were predicted by TD-DFT methods and measured experimentally, which facilitated the determination of the stoichiometry and formation constant of the Fe(II)-gallic acid coordination compound through the Job plot construction.[4,5] The deprotonation order and corresponding microscopic pKa values of 4 investigated ellagitannins were determined using ^{13}C NMR spectroscopy as well as subsequently applied to elucidate the mechanistic model of the formation of their coordination compounds with Fe(II).[6] Last but not least, the advanced ICP-OES technique was used to determine the amount of essential metal ions in *E. Coli* cells in the presence/absence of the investigated ellagitannins.

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COHERENT VIBRATIONAL WAVE-PACKETS IN SINGLET FISSION – THEORETICAL MODELING OF THE IMPULSIVE VIBRATIONAL SPECTRA

Marcin Andrzejak[a], Grzegorz Mazur[b], Andrew J. Musser[c], Piotr Petelenz[d], Tomasz Skóra[e]

[a] K. Gumiński Department of Theoretcal Chemistry, Facuty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland; m.andrzejak@uj.edu.pl

[b] Department of Computational Methods in Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland; mazur@chemia.uj.edu.pl

[c] Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853, USA; ajm557@cornell.edu

[d] K. Gumiński Department of Theoretcal Chemistry, Facuty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland; petelenz@chemia.uj.edu.pl

[e] Scientific Computing and Imaging Institute, University of Utah; tskora93@gmail.com

Singlet fission (SF) has attracted increasing attention in the recent years due to the putative application of this phenomenon to increase the efficiency of optoelectronic devices by amplifying the number of charge carriers obtainable from a single photon. The essential objective is to rationalize the fundamental mechanisms of singlet fission and pinpoint the characteristics of chromophores that would be optimal for this purpose.

The singlet fission process lasts from several to several tens of femtoseconds, so it requires ultrafast techniques of investigation, such as the impulsive vibrational spectroscopy (IVS), in which the pumping step, effected by a femtosecond coherent light pulse (10–20 fs), promotes the chromophore from its ground state (S_0) to the first excited singlet state (S_1). Concurrently it generates nonstationary vibrational wave packets, which are smoothly transferred onto the potential energy surface of the entangled triplet pair state ^{1}(TT), where they are detected by a second laser pulse. The assumption that the vibrational wave packets are unaffected by change of the electronic state, however, needs to be verified, especially in view of the claim put forth by Stearn at al. that coherent wave packets may be generated by the fission process itself [1].

We propose a phenomenological wavefunction-based model of vibrationally coherent absorption modulation [2,3] and apply it to reproduce the IVS spectra of two different, pentacene related systems [1,4], with the objective of testing whether the singlet fission process in that system spontaneously generates coherent vibrational packets or it is neutral with respect to vibrational coherences.

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STEERING EXCITED STATE PROTON TRANSFER: AN INTERPLAY OF ELECTRONIC AND STRUCTURAL FACTORS

Nađa Došlić

[a] Ruđer Bošković Institute, Bijenička c. 54, 10000 Zagreb, Croatia
nadja.doslic@irb.hr

Excited-state proton transfer (ESPT) reactions typically occur between a proton donor (e.g., NH or OH) and an electronegative heteroatom.[1] Sometimes, however, the proton acceptor can be a carbon atom.[2] In 2002, Wan et al. reported the first example of direct photoprotonation of a carbon atom of an aromatic ring via excited-state intramolecular proton transfer (ESIPT).[3] At first glance, ESPT to a carbon atom is somewhat surprising, since protonation of an aromatic carbon atom typically is a slow process in the ground state. Yet, why do some aromatic ring carbons gain basicity in the excited-state?

Excited-state antiaromaticity relief can play important roles in many light-driven proton and electron transfer reactions. Here, we report on the photo-protonation mechanism of three aminobiphenyl isomers.[4] In all three cases, a proton formally migrates from an NH2 group to an aromatic ring carbon atom. All three isomers, ortho-, meta-, and para-, can undergo ESPT involving water. In addition, the meta-isomer can undergo a photoredox reaction, involving proton-coupled electron transfer and water-splitting. We suspect that strong antiaromaticity in the aniline ring may be responsible for driving the observed reactions.

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GEOMETRIC ALGEBRA APPROACHES TO PROTEIN-PROTEIN DOCKING

Azzam Alfarraj,[a] Guo-Wei Wei,[b,c,d]

[a] Mathematics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, KSA
azzam@kfupm.edu.sa
[b] Department of Mathematics, Michigan State University, MI 48824, USA
weig@math.msu.edu
[c] Department of Biochemistry and Molecular Biology, Michigan State University, MI 48824, USA
[d] Department of Electrical and Computer Engineering, Michigan State University, MI 48824, USA

(Geometric algebra is a powerful framework that unifies mathematics and physics. Since its revival in the 1960s, it has attracted great attention and has been exploited in fields like physics, computer science, and engineering. Its potential has yet to be leveraged in biology and biochemistry. This work introduces geometric algebra methods for protein-protein docking and molecular surface generation. The first method utilizes rotors for rotations instead of rotation matrices, exploiting the efficiency and compactness of geometric algebra operations. This approach reduces the number of operations needed significantly. The proposed method, GADOCK, was assessed on 36 enzyme-inhibitor pairs from the Protein Docking Benchmark and compared to the FMFT method. GADOCK outperforms FMFT in terms of execution time, accelerating the local search stage by 15% on average, noting that this stage is by far the most expensive stage in the docking process, accounting for 90%. On top of that, this efficiency enhancement was not in the trade of accuracy. Both methods produce very comparable case-by-case results, and GADOCK performs better on average, improving the accuracy by 8.42% when averaged over all pairs and 19.82% when averaged over good predictions only. The accuracy was measured using interface $C\alpha$ RMSD)

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RELIABLE DESCRIPTION OF LARGE ORGANIC MOLECULES WITH PCCD-BASED METHODS

Paweł Tecmer

Institute of Physics, Nicolaus Copernicus University in Toruń, ptecmer@fizyka.umk.pl

The efficiency of organic solar cells (OSCs), typically composed of conjugated polymers as donors and fullerene derivatives as acceptors, is strongly related to their structure-property relationship. Example factors that play an essential role in the design of more efficient OSCs are the conformation of frontier molecular orbitals, the offset between the donor's highest occupied molecular orbital and the acceptor's lowest unoccupied molecular orbital, characteristic features of low-lying electronic transitions, and dipole moments. Unfortunately, OSCs' molecular size and building blocks prohibit us from employing the most accurate state-of-the-art quantum chemistry methods. During this talk, I will discuss how we can use the pair coupled-cluster doubles (pCCD)-based approaches [1] to model electronic structures and properties of OSC building blocks efficiently and reliably [2,3]. These include (a) computation of orbital energies, (b) dipole moments, (c) the static pCCD-in-DFT embedding approach [4], and (d) the linear response pCCD-based models.

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IMPROVED EVALUATION METRICS OF CLASSIFICATION AND LANGUAGE MODELS IN CHEMISTRY AND BEYOND

Bono Lučić[a], Viktor Bojović[b], Antonija Kraljević,[c] and Jadranko Batista[d]

[a] Ruđer Bošković Institute, NMR Centre, Zagreb, Croatia, lucic@irb.hr
[b] Ruđer Bošković Institute, Centre for Informatics and Computing, Zagreb, Croatia
[c] University of Mostar, Faculty of Mechanical Engineering, Computing and Electrical Engineering, Mostar, Bosnia and Herzegovina
[d] University of Mostar, Mostar, Faculty of Science and Education, Bosnia and Herzegovina

Classification models are developed and used in chemistry, but also in all other areas of science, technology and industry [1]. Their use has greatly accelerated due to the great advances in artificial intelligence (AI) technology that we have witnessed in recent years [2]. Although Large Language Models (LLMs) temeljeni na algoritmu Tranformer have shown strong performance on tasks in various domains, they still struggle with the specificity of chemical information and the lack of access to external knowledge sources [3]. However, LLMs are expected to be increasingly used in science, including chemistry. Their quality is evaluated using specific metrics that only partially match the metrics used to evaluate general classification models [2]. Another problem is the evaluation of algorithms for recognising patterns in images when trying to develop an AI tool/model for reading medical imaging findings [4]. Accuracy, F1-score, AUCROC (Area under the ROC Curve) [1] and MCC (Matthew's Correlation Coefficient) [5] and sometimes Cohen's Kappa [6] have long been used as metrics in the literature. Recently, the use of the model evaluation metric MCC has been favoured for classification models [7]. This problem is particularly pronounced in the area of modelling and recognition of patterns in images, which is especially important when trying to automatically read image findings in medical applications [4]. The properties and interpretations of the most commonly used metrics based on the elements of the Confucian matrix and their mutual relationships have been investigated. In order to evaluate the real progress in the development of classification models and to improve metrics used to evaluate the quality of classification and LLMs models, it is necessary to define objective measures of model quality that measure the progress achieved compared to random guessing (random model) [8]. At the same time, the nature of the problem to be modelled and the balance of the error with respect to the distribution of classes in the experimental data and in the prediction obtained by the model must be taken into account.

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THE HITCHIKER'S GUIDE TO THE WAVEFUNCTION

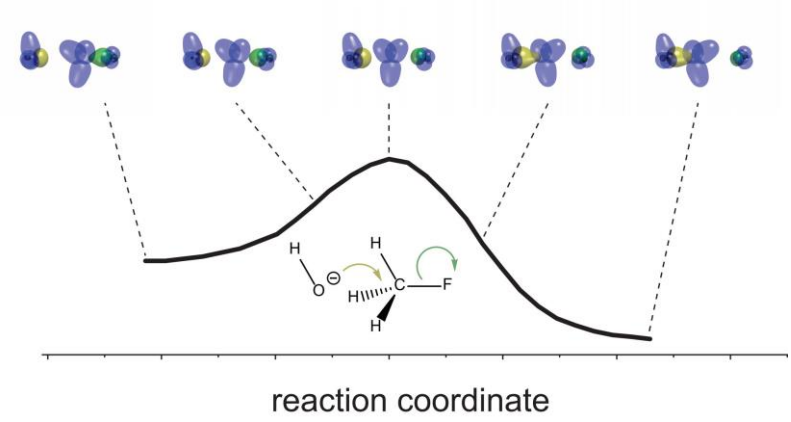
Yu Liu,[a] Timothy W. Schmidt,[b] Philip Kilby[c] and Terry J. Frankcombe[d]

[a] Shanghai University, Shanghai, China; z3386640@zmail.unsw.edu.au
[b] University of New South Wales, Sydney, Australia; timothy.schmidt@unsw.edu.au
[c] Data 61, Canberra, Australia; philip.kilby@data61.csiro.au
[d] University of New South Wales, Sydney, Australia; t.frankcombe@adfa.edu.au

Schrödinger's wave mechanics is a very successful formulation of quantum mechanics, built around the wavefunction. Wavefunctions are single valued functions that inherently inhabit high dimensional spaces and contains all of the information about a quantum system that is possible to know.

Over a number of years, we have been developing a method of interrogating multielectron wavefunctions in order to reveal their high dimensional structure [1–7]. Our approach relies on the indistinguishability of fundamental particles, which implies that the entire information content of the wavefunction for N interacting particles that in principle fills 3N dimensional space can be reduced to the value of the wavefunction on a slice of this space. The entire wavefunction can be reproduced by replicating the wavefunction from this slice onto other slices of the space by relabelling the coordinates, possibly with a sign change. In other words, the high dimensional wavefunction is inherently built in a tiling of 3N space. The structure of a self-consistent tiling gives insight into the structure of the full dimensional wavefunction.

We call this method the Dynamic Voronoi Metropolis Sampling (DVMS) method, as it relies on a weighted random walk of a population of Monte Carlo points, constrained in part by a Voronoi decomposition of the 3N space. In this talk I will give an overview of our work to date.



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WORKSHOP

SPECIAL TOPICS IN THE THEORY OF ANGULAR MOMENTUM

Henryk A. Witek

Department of Applied Chemistry and Institute of Molecular Science, National Yang Ming Chiao Tung University, Hsinchu 30010, Taiwan, hwitek@nycu.edu.tw

A typical curriculum of a quantum chemist includes a course covering some elements of angular momentum theory. In most cases, such a course covers the quantization of angular momentum, the representation of the operators in spherical coordinates, the resulting theory of spherical harmonics, the algebraic theory of angular momentum based on the commutators, and the Clebsch-Gordan addition of two angular momenta. Many interesting advanced topics, such as angular momentum in higher dimensions, addition of a larger number of angular momenta (including 6-*j* and 9-*j* symbols), Racah theory of complex spectra, angular momentum theory of rigid and non-rigid bodies, accidental degeneracies and the dynamical symmetries are seldom included in the course work and most students and scientists familiar with these concepts usually learn them only by active research in this field.

The current short course is supposed to familiarize the participants with two semi-advanced topics in the theory of angular momentum, the theory of Wigner *D* functions corresponding to the wave function of a rotating rigid body in 3D, and the Fock approach accounting for the accidental degeneracy in the energy spectrum of the hydrogen atom. Both topics will be presented in an elementary fashion, without assuming any deep knowledge of the theory of angular momentum. It is hoped that such an elementary exposition will demystify these concepts, which are often deemed as difficult and non-accessible to a non-specialist.

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POSTERS

USING NUMERICAL TENSOR METHODS FOR SOLVING THE MANY-BODY SCHRÖDINGER EQUATION

Kammegne T. Brice[a], Michael Melgaard,[b] and Hazel Cox[c]

[a] Department of Chemistry & Mathematics, University of Sussex, Brighton BN1 9QJ, U.K; K.Brice@sussex.ac.uk
[b] Department of Mathematics, University of Sussex, Brighton BN1 9QJ, U.K; M.Melgaard@sussex.ac.uk
[c] Department of Chemistry, University of Sussex, Brighton BN1 9QJ, U.K; H.Cox@sussex.ac.uk

The continuous expansion of computing power has led to new attempts at solving well known problems with increasing numerical accuracy at reduced computational cost. Among these challenges, the all-particle treatment of three-body atoms and molecules stands out as an ideal test case for evaluating new methods. Numerical tensor methods (NTM) have emerged as a powerful technique for efficiently representing and manipulating high-dimensional data in various scientific disciplines. In this work, we use NTM to approximate the solution of the Schr¨odinger equation (SE) for three-body atoms and molecules. Using perimetric coordinates, the SE is first recast in a canonical tensor format, and the wave function is approximated as a linear combination of Lagrange polynomials, discretized using Chebychev nodes. Employing the Galerkin formulation, the SE is represented in full, tensor train (TT) and quantised tensor train (QTT) formats. It will be shown that, in full tensor format, we can achieve energies accurate to at least the nano-Hartree for the He atom and the positronium negative ion Ps^-, and at least micro-Hartree accuracy for the non-BO H_2^+ molecule. However, in TT and QTT formats, high quality wave functions, and energies accurate to greater than a nano-Hartree, can be achieved for all the types of system considered (atomic, exotic and molecular) using smaller computational resources.

REACTION REBALANCING: A NOVEL APPROACH TO CURATING REACTION DATABASES

Tieu-Long Phan,[1,a] Klaus Weinbauer,[2,a] Peter F. Stadler[3,a]

[a] Bioinformatics Group, Department of Computer Science & Interdisciplinary Center for Bioinformatics, Leipzig University, Härtelstraße 16–18, D-04107 Leipzig, Germany.

[1] tieu@bioinf.uni-leipzig.de

[2] klaus@bioinf.uni-leipzig.de

[3] studla@bioinf.uni-leipzig.de

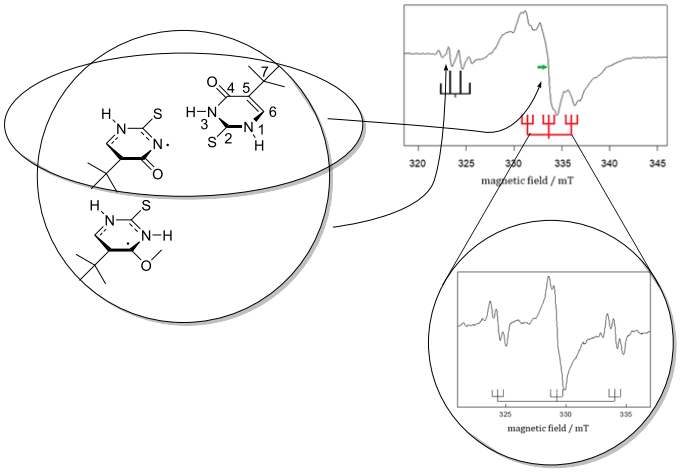
Reaction databases are an essential resource for various computational chemistry and biochemistry applications, including Computer-aided Synthesis Planning (CASP) and the large-scale analysis of metabolic networks. The full potential of these resources can only be realized if data sets are accurate and complete. However, missing co-reactants and co-products, i.e., unbalanced reactions, are the rule rather than the exception. The SynRBL framework addresses this issue with a dual strategy: a rule-based method for imputing non-carbon compounds using the atomic composition alongside a maximum common substructure (MCS)-based technique aligning reactants and products to infer missing carbon structures. The overall efficacy of this framework was delineated through its success rate and accuracy metrics, which spanned from 89.83% to 99.75% and 90.85% to 99.05%, respectively. SynRBL offers a novel solution for recalibrating chemical reactions, significantly enhancing reaction completeness.

A QUANTUM CHEMICAL INSIGHT INTO RADICAL REARRANGEMENTS IN THE SINGLE CRYSTAL OF 2-THIOTHYMINE

Gabrijel Zubčić, Valerije Vrček, Viktor Pilepić, Davor Šakić and Erim Bešić

University of Zagreb, Faculty of Pharmacy and Biochemistry, Ante Kovačića 1, 10000 Zagreb, Croatia
gzubcic@pharma.hr

Thionucleobases exhibit a distinct feature when compared to their canonical equivalents and that is the shift of the absorption spectra from the UVC area into the UVA region (320-400 nm). Because of this unique absorption characteristics, thionucleobases can be selectively photoactivated into the electronic triplet state.[1–3] In triplet state homolytic cleveage of N-H bond can occur. This study sheds light on EPR experiments comprising gamma irradiation of 2-thiothymine crystals, a nucleobase analogue, under varying thermal conditions (77 K and 300 K). The irradiation process furnishes two distinct radical pair species at these temperatures. At 100 K, upon gamma-ray-induced cleavage of N_3-H bonds, two radicals are formed. Their formation is facilitated by inter- or intra-layer hydrogen atom transfer, with strong interactions with nearby molecules inside crystal structures. The transition to more stable radicals at elevated temperatures involves further interlayer rearrangements, as rate constant increases dramatically when temperature is elevated from 100 to 300K. This research not only investigates the stability and transformation mechanisms of radiation-induced radicals in nucleobase analogues but also provides a framework for understanding the thermodynamics and kinetics underpinning these processes.



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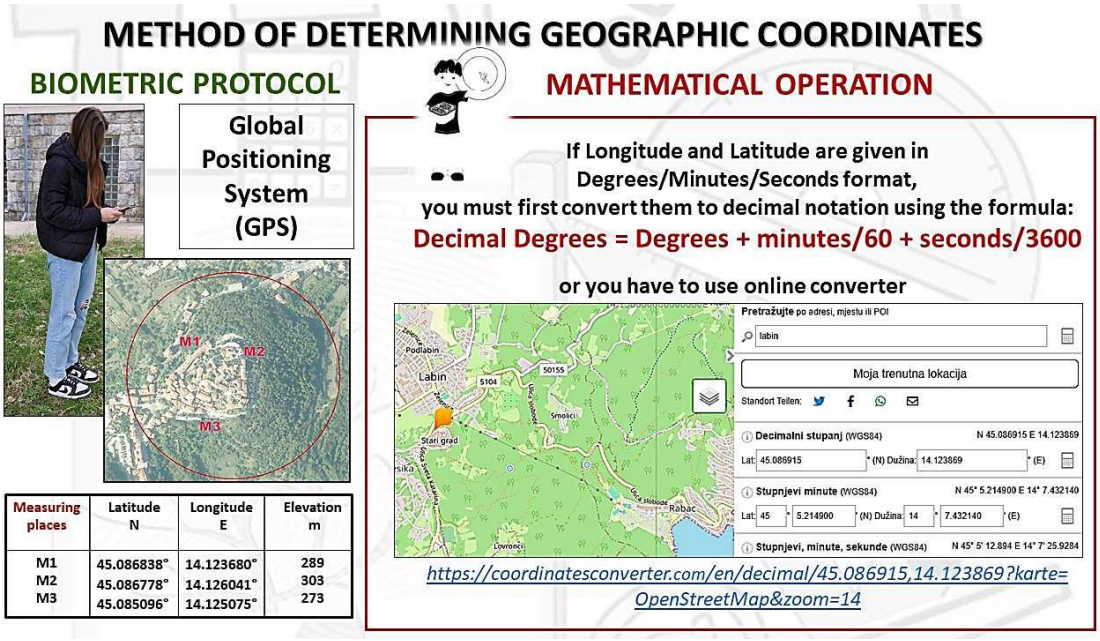
DO BIOMETRIC MEASUREMENTS OF TREES NEED MATHEMATICS?

Olivera Tadić & group of students

Srednja škola Mate Blažine Labin, Rudarska 4, 52220 Labin, Croatia
ekolja@gmail.com

Within the framework of the school program "SCHOOL FOR THE ENVIRONMENT" (already 46 years) and THE GLOBE PROGRAM (already 26 years) we pay special attention to student research project.

All works are available on the school's website, *https://ssmb.hr/*, the Globe program website: *https://www.globe.gov/do-globe/research-resources*, or You tube channel: *https://www.youtube.com/results?search_query=olivera+tadi%C4%87*, and are also published in local media.



Measuring places	Latitude N	Longitude E	Elevation m
M1	45.086838°	14.123680°	289
M2	45.086778°	14.126041°	303
M3	45.085096°	14.125075°	273

RARE-EARTH HIGH-ENTROPY OXIDES – DRIVEN ENHANCEMENT OF CERIA'S PHOTOCATALYTIC WATTER SPLITTING: EXPERIMENT AND DFT STUDY

Igor Djerdj,[a] Stjepan Šarić,[a] Dalibor Tatar,[a] Jelena Kojčinović,[a] Ronen Gottesman,[b] Oded Millo,[c] Doron Azulay,[d] Habib Ullah[e]

[a] Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, 31000 Osijek, Croatia, igor.djerdj@kemija.unios.hr

[b] Institute of Chemistry, The Hebrew University of Jerusalem, Edmond J. Safra Campus, Givat Ram, 9190401 Jerusalem, Israel.

[c] Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Edmond J. Safra Campus, Givat Ram, 9190401 Jerusalem, Israel.

[d] Department of Physics, Azrieli College of Engineering Jerusalem, POB 3566, 9103501 Jerusalem, Israel.

[e] Environment and Sustainability Institute, University of Exeter, Penryn TR10 9FE, United Kingdom.

Five different rare-earth-based high-entropy oxides (HEOs) in nanocrystalline form were synthesized using a modified aqueous sol-gel route.[1] All examined HEOs represent equimolar 5-cation system selected from the elements: Ce, Zr, La, Pr, Gd, Eu, Y that were uniformly distributed and demonstrated a single fluorite structure with lattice parameter similar as parent simple oxide CeO_2. The variation of equimolar chemical composition yielded the band gap variation and modulation of electronic structure. Among studied HEOs, $Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Y_{0.2}O_2$ (CZLPY) has shown the highest photocatalytic activity in AZO dyes degradation and photocatalytic water splitting in hydrogen generation than any other synthesized HEOs due to the presence of optimum level of Pr^{3+}, Ce^{3+} and the highest content of oxygen vacancies as verified by XPS. Thus, the phase stabilisation of high-entropy oxide in parent CeO_2 lattice induced more lattice distortion, more Ce^{3+} concentration, more oxygen vacancies and additional energy levels (due to more oxidation states of Ce and Pr) as compared to pure CeO_2. According to the DFT calculations, the most appropriate model of the crystal structure of CZLPY is the one where O anions are tetrahedrally coordinated with four different (Ce, La, Zr, Pr, Y) cations. The most stable fluorite surface along [111] is verified as a model/catalyst for Zr, La, Pr, and Y dopants, followed by the interaction with water and MB molecules. Based on experimental findings and theoretical modelling, this work provides a significant step for enhancing the photocatalytic performance of rare-earth-based HEOs.

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A SENSITIVITY ANALYSIS OF THE FORMOSE CHEMISTRY WITH BORATE USING RULE-BASED STOCHASTIC SIMULATIONS

Erika M. Herrera Machado[a], Jakob L. Andersen[a], Rolf Fagerberg[a], Daniel Merkle[a,b]

[a] Department of Mathematics and Computer Science, University of Southern Denmark, Odense DK-5230, Denmark
[b] Faculty of Technology, Bielefeld University, Bielefeld, Germany
machado@imada.sdu.dk; jlandersen@imada.sdu.dk; rolf@imada.sdu.dk; daniel@imada.sdu.dk

In this study, we conduct a derivative-based local sensitivity analysis in order to explore the formose chemical system in the presence of borate. Our work builds upon the prior study in [2], where they discuss the role of borate in the guidance and moderation of the formose process, leading to the selective formation and stabilization of pentoses and pentuloses – essential five-carbon sugars with significant implications for genetic systems. A chemical rule-based system is defined, and network-free stochastic simulations are performed using the software package MØD [1] for graph-based cheminformatics. We will examine how our results correlate with the hypotheses outlined in the experiments in [2].

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MOLECULAR DESCRIPTORS BASED ON AUTOMORPHISM DATA

Kurt Varmuza,[a,b] Matthias Dehmer,[c,d] and Peter Filzmoser[a]

[a] Vienna University of Technology, Institute of Statistics and Mathematical Methods in Economics, Computational Statistics, Wiedner Hauptstrasse 7/105-6, A-1040 Vienna, Austria
kurt.varmuza@tuwien.ac.at; peter.filzmoser@tuwien.ac.at

[b] Vienna University of Technology, Institute of Chemical, Environmental and Bioscience Engineering, Getreidemarkt 9/166-2, A-1060 Vienna, Austria

[c] Swiss Distance University of Applied Sciences, Department of Computer Science, Schinerstrasse 18, CH-3900 Brig, Switzerland; matthias.dehmer@ffhs.ch

[d] UMIT TIROL - Private University For Health Sciences and Health Technology, Eduard Wallnöfer Zentrum 1, A-6060 Hall in Tyrol, Austria

Chemical structures are represented by colored mathematical graphs with vertices (atoms) defined by one of three elements (C, N, O), and edges (bonds) defined by one of four bond types (single, double, triple, aromatic). The complete automorphism group [1] of such chemical structure graphs is determined [2,3] and then evaluated by functions in the programming environment R [4].

Molecular descriptors based on automorphism data comprise symmetry and entropy measures, as well as roots of graph polynomials. For instance, the orbit polynomial [5] has been defined by orbit data for vertices and edges obtained from the automorphism data of graphs. In a previous work this concept was applied to exhaustive sets of isomeric alkanes [6] and is now extended to coloured graphs (CHNO molecules). Such descriptors have been used here together with already common ones for the creation of models for quantitative structure property relationships and for the prediction of chemical class memberships. Multivariate calibration models have been obtained by linear PLS regression optimized and evaluated by the strategy repeated double cross validation [7,8].

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CHEMICAL ORGANISATIONS IN STOCHASTIC RARE EVENT SIMULATIONS OF RULE-BASED CHEMICAL SYSTEMS

Deza Amistas,[a] Christoph Flamm,[b] and Peter Dittrich[c]

[a] Department of Mathematics and Computer Science, Friedrich Schiller University Jena, Jena, Germany
deza.amistas@uni-jena.de
[b] Institute of Theoretical Chemistry, University of Vienna, Wien, Austria
xtof@tbi.univie.ac.at
[c] Department of Mathematics and Computer Science, Friedrich Schiller University Jena, Jena, Germany
peter.dittrich@uni-jena.de

A chemical reaction system is a system composed of chemical molecules that react with each other. A set of chemical molecules that is closed and self-maintaining is called an organisation. An organisation can tell which systems can exist for a long time. Several methods have been developed over the years to understand and predict the dynamics of chemical reaction systems, and among them is the Gillespie algorithm. The Gillespie algorithm uses stochastic approach to describe the state of a well-stirred chemically reacting system after some time. Unlike the deterministic approach, the stochastic approach takes into consideration the randomness in the behavior of molecules, making the results more robust. Considering the reactions that happen in a well-stirred environment, a specific organisation can be observed after some time where no new molecules are being added or lost. However, there is a possibility that a chemical organisation can transition into another chemical organisation, and such event is called a rare event. Although a rare event has a very small probability of occurring, it can greatly affect the behavior of the reaction system. It can either create a bigger organisation, causing an explosion in the reaction system, or it can eliminate some molecules that can eventually lead to the demise of the whole system. We aim to better understand the dynamics of such complex systems. We also aim to propose new methods on how to deal with these systems using the idea of organisation theory while incorporating rare events in stochastic simulations.

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AUTHORS AND PARTICIPANTS

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Alfarraj, Azzam 50
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Boguslawski, Katharina
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Bubin, Sergiy
Camacho, Cristopher
Cioslowski, Jerzy
Cocut, Andrea
Cox, Hazel
Dale, Stephen
Djerdj, Igor
Došlić, Nadja
Došlić, Tomislav
Frankcombe , Terry
Gladbach, Lena
Herbert, John
Herrera Machado, Erika
Iranmanesh, Ali
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Jakobsen, Patrick
Karwowski, Jacek
Klein, Douglas J. Klein
Komasa, Jacek
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Maitra, Rahul
Melgaard, Michael
Namjesnik, Danijel
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Phan, Tieu-Long
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Savin, Andreas
Shrikhande, Chinmay
Solà, Miquel
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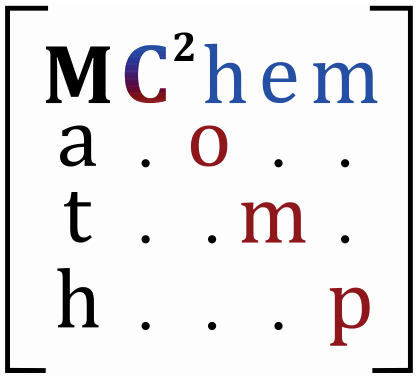

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