13th VISEGRAD SYMPOSIUM ON BIOMOLECULAR INTERACTIONS

PROGRAM & ABSTRACTS

18th– 21st June 2025

Ostravice

Czech Republic

Organization

VSB TECHNICAL UNIVERSITY OF OSTRAVA
IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

Scientific Orginizing Committee:

Babak Minofar, University of Miskolc, Hungary; University of Łódź, Poland
David Řeha, VŠB Technical University of Ostrava, Czech Republic
Milan Melicherčík, Comenius University in Bratislava, Slovakia
Béla Viskolcz, University of Miskolc, Hungary
Marcin Palusiak, University of Łódź, Poland
Christian Schröder, University of Vienna, Austria

Local Organizing Team

David Řeha
Zuzana Červenková
Barbora Poláková

Inivited Speakers

Jannette Carey, Princeton University, NJ, USA
Johannes Dietschreit, University of Vienna, Austria
Maren Podewitz, Technical University of Vienna, Austria
Sarah Harris, University of Sheffield, UK
Nacer Idrissi, University of Lille, France
Jocelyne Vreede, University of Amsterdam, Netherlands
Dominik Horinek, University of Regensburg, Germany
Jeanine J. Houwing-Duistermaat, Radboud University, Nijmegen, Netherlands
Bela Viskolcz, University of Miskolc, Hungary

Symposium program

Wendsday, June 18

15.00-17.00	**Registration**
17.00-17.10	**Conference opening**

Chairperson: Christian Schröder

17.10-17.40	**Maren Podewitz (Wien)**: Supramolecular Chemistry: Machine Learning and Causality to Reveal the Reaction Coordinate
17:40-18:10	**Johannes Dietschreit (Wien)**: Calculating Free Energies without Approximations
18:10-18:40	**Denés Berta (Budapest)**: Towards accurate simulations of enzymatic reactions
18:40-19:00	**Marion Sappl (Wien)**: Terahertz spectroscopy of supercritical water – a molecular dynamics approach

19.00-	**Poster session, welcome party**

Thursday, June 19

Chairperson: Sarah Harris

09:00-09:30	**Jannette Carey (Princeton)**: Predicting ligand binding in the age of big data
09:30-10.00	**Jocelyne Vreede (Amsterdam)**: Modeling protein-DNA interactions
10:00-10:20	**Christian Fellinger (Wien)**: GRADE-ing Protein-Ligand Interactions
10:20-10:40	**Khalida Khalil (Łódź)**: Computational Approaches to Molecular Interactions in Inclusion Complexes of Calix[n]arenes

10:40-11:10	Coffee break

Chairperson: Jeanine Houwing-Duistermaat

11:10-11:40	**Sarah Harris (Sheffield)**: From genes to machines - multiscale biomolecular simulations
11:40-12:10	**Zsófia Borbála Rózsa (Miskolc)**: Effect of phospholipid headgroups on the membrane penetration of NSO-HET compounds
12:10-12:30	**Nesreen Alkanakri (Miskolc)**: Experimental and Computational Insights into Electrospinning Solutions of PVA, Chitosan, and Collagen
12:30-15:50	**Tamás Horváth (Miskolc)**: Thermodynamics of Decorporol complexes with Sr^{2+} and Ca^{2+} ions - A combined Isothermal titration Calorimetry and DFT Study

13:00-14:00	**Lunch**
14:00-19:30	**Free time, individual trips and excursions**
19:30-	**Dinner, BBQ**

Friday, June 20

Chairperson: Jannette Carey

09:00-09:30	**Jeanine Houwing-Duistermaat (Utrecht)**: Principal Components Modelling of Longitudinal Omics Dat
09:30-10:00	**Agnieszka Rybarczyk-Pirek (Łódź)**: Studies on low-barrier N^+–H…O^- hydrogen bond in pyrimidine–carboxylic acids multicomponent crystals
10:00-10:20	**Patryk Czapnik (Łódź)**: New chromone analogues condensed with 1,2,3-triazoles
10:20-10:40	**Olga Książkiewicz (Łódź)**: Research towards synthesis of multicomponent crystals consisting of biologically active components
10:40-11:10	Cofee break

Chairperson: Jocelyne Vreede

11:10-11:40	**Dominik Horinek (Regensburg)**: ATP-peptide interactions And Peptide Aggregation
11:40-12:10	**Jaroslav Burda (Prague)**: Interactions in models of Thioredoxin reductase; DFT & QM/MM studies
12:10-12.40	**Christian Schröder (Wien)**: Advancing Proton Transfer Simulations in Ionic Liquids
12:50-14:00	**Lunch**

Chairperson: Béla Viskolcz

14:00-14:30	**Milán Szőri (Miskolc)**: Atomistic Simulations for Sustainable Chemistry and Environmental Safety: From Chlorine Storage to PFAS–Plastic Interactions
14:30-15:00	**Béla Fiser (Miskolc)**: Making and breaking polyurethanes
15:00-15:20	**Peter Koska (Miskolc)**: Biosorption and Bioaccumulation of Nickel by Chlorella vulgaris microalga
15:20-15:40	**Dalal K. Thbayh (Miskolc)**: Computational and Experimental Study of Antioxidant Polymer Additives
15:40-16:10	Coffee break

Chairperson: Marcin Palusiak

16:10-16:40	**Béla Viskolcz (Miskolc)**: Biological removal of heavy metals from water
16:40-17:10	**Rehana Bano (Miskolc)**: Designing the Future of Photonics: Superalkali-Based Electrides and Alkalides for Enhanced Nonlinear Optical Response
17:10-17:30	**Julie Malouhi (Miskolc)**: Ecotoxicological Assessment of Polyurethane Foams and Bio-Based carbonaceous Materials: Environmental Impacts and Applications
17:30-18:00	**Closing remarks**
19:00-	**Conference diner, farwall party**

Saturday, June 21: Departure

List of posters

1. **Lilianna Chęcińska (Łódź):** Symmetric O···H···O and asymmetric O-H···O hydrogen bonds in multicomponent crystals of pyridinedicarboxylic acids
2. **Małgorzata Domagała (Łódź)**: New polymorph of methyl 3,4-dicyano-1-methyl-2,5-diphenylpyrrolidine-3-carboxylate
3. **Tímea Gerzsenyi (Miskolc)**: Plasmon-Enhanced Fluorescence Analysis of DNA Origami Immobilized on Gold Nanoparticles
4. **Adnan M. Khan (Miskolc)**: Multifunctional Polyurethane Foams: Influence of Ag_2O Doping on Structural and Functional Properties
5. **Nuša Matjašec (Wien)**: Computational Characterization of LPS Membranes and Their Interaction with Alternariol
6. **Milan Melicherčík (Bratislava)**: Overview of potassium channel selectivity filter occupancy by K^+ ions and water molecules
7. **Ewa Muzal (Łódź)**: Thermal Characterization of Paraffin Candles Modified with Dyes and Fragrances Using DSC
8. **Aleksndra Rydz (Łódź)**: Analysis of superstrong hydrogen bonds in thiourea complexes
9. **Marcin Wlaźlak (Łódź)**: The impact of visible light and darkroom conditions on the crystallization of systems containing trithiocyanuric acid
10. **Kinga Wzgarda-Raj (Łódź)**: Hydrogen bonding patterns in trithiocyanuric acid cocrystals: structural, topological, and energetic analysis into N–H···S interactions

Abstracts of oral presentations

The authors of the abstracts bear the full responsibility for the scientific and linguistic content.

Supramolecular Chemistry: Machine Learning and Causality to Reveal the Reaction Coordinate

Maren Podewitz

Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060 Vienna, Austria

Supramolecular catalysts based on abundant first row transition metals offer a sustainable alternative to precious metals in key bond-forming reactions. However, the flexible nature of these macrocyclic systems presents a significant challenge to quantum chemical modeling.

I will report a recently developed multiscale protocol that elucidates the mechanism of C–N coupling catalyzed by a Cu–calixarene complex. To capture the dynamics of C–N bond formation, we used a quantum mechanics/molecular mechanics (QM/MM) molecular dynamics (MD) protocol in an explicit chloroform environment, producing over 150 trajectories of this reaction step. To analyze these data we utilized interpretable machine learning techniques for feature selection in a consensus model and applied, for the first time, a Granger causality model to redefine the reaction coordinate as a sequence of molecular motions.

Calculating Free Energies without Approximations

Johannes Dietschreit

University of Vienna, Faculty of Chemistry, Institute of Theoretical Chemistry

Describing chemical processes at the molecular level often relies on the use of reaction coordinates or collective variables (CVs), which track the progress of a reaction and enable the construction of profiles that reflect the evolution of specific properties. For a reaction proceeding from reactants (R) to products (P) on a potential energy surface (PES), and a CV capable of distinguishing between R and P, the potential of mean force (PMF) is defined as the logarithm of the marginal Boltzmann distribution of the CV.

Despite its widespread use, the PMF is frequently (and misleadingly) interpreted as a “free-energy” analog of the minimum energy path, due to its apparent resemblance to the PES along the R–P transformation. However, because the PMF depends functionally on the chosen CV, it can assign different values to the same configurations in Cartesian space, leading to inconsistencies. As such, the PMF generally does not represent a true free energy profile. We show that this common interpretation can lead to significant errors.

In this work, we derive tractable expressions for the free energy, internal energy, and entropy profiles as functions solely of the CV [1]. We present simple and exact formulations for reaction [2] and activation [3] energies and entropies, which—unlike the PMF—do not share its dependence on the CV's specific form. We illustrate how this framework enables the extraction of quantitative insights from entropy and energy profiles in realistic physicochemical processes, including intramolecular organic reactions.

[1] Dietschreit, J. C. B.; Diestler, D. J.; Gómez-Bombarelli, R. Entropy and Energy Profiles of Chemical Reactions. J. Chem. Theory Comput. 2023, 19(16), 5369-5379

[2] Dietschreit, J. C. B.; Diestler, D. J.; Ochsenfeld, C. How to obtain reaction free energies from free-energy profiles. J. Chem. Phys. 2022, 156(11), 114105

[3] Dietschreit, J. C. B.; Diestler, D. J.; Hulm, A.; Ochsenfeld, C.; Gómez-Bombarelli, R. From free-energy profiles to activation free energies. J. Chem. Phys. 2022, 157(8), 084113

Towards accurate simulations of enzymatic reactions

Denes Berta[1,2], Jozsef Csoka[2], Bence Hegely[2], Peter R. Nagy[2]

[1]Department of Physical Chemistry and Materials Science, Budapest University of Technology and Economics, Műegyetem rkp. 3, Budapest 1111, Hungary
[2]Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom

berta.denes@bme.vbk.hu

Beginning with the seminal work of Karplus, Levitt and Warshel, the main compu- tational tool for modelling of biochemical reactions is the hybrid Quantum Mechanics – Molecular Mechanics (QM/MM) framework. This multiscale approach leverages the strengths of different levels of particle models: QM methods are used to describe the chemistry in an active site, MM is capable of treating huge systems describing a non- reactive, anisotropic atomistic environment in the protein.

However, QM/MM is arguably one of the most technically difficult computational scheme, due to the various choices and parameters that need choosing: QM theory, basis set, MM force field, selection of the QM region, description of the interface, sampling method, and so on. All of these aspects have seen serious developments in the last decades and we know much of the convergence of simulated properties with an individual parameter, while the rest are kept at a reasonable value [1].

We aim to face the entanglement of QM/MM simulation parameters and employ ad- vanced QM techniques to establish a multi-dimensional sweet spot for enzymatic reactions. We explore the convergence of reaction barriers and energies for a representative phos- phate catalytic enzyme, the Ras GTPase [2], exhibiting a number challenges for widely used DFT methods. We observe varying error cancellation with different QM regions and basis sets and establish minimum requirements for a robust model. From testing multiple QM selection algorithms, we establish key principles and recognise no one-for-all approach exists. To enable free energy calculations for experimental comparison, we further divide the QM region and test ONIOM and Huzinaga embedding schemes [3] achieving stellar simulation speed-up maintaining accuracy.

Overall, we demonstrate both the importance and the applicability of the combination of cutting-edge methodology in QM/MM modelling, encouraging the community to use such tools developed by us [4] and others.

[1] Vennelakanti, V.; Nazemi, A.; Mehmood, R.; Steeves, A.H. and Kulik, H.J.; *Curr. Opin. Struct. Biol.*, **2021**, *72*, 9–17.
[2] Berta, D.; Gehrke, S.; Ny´ıri, K.; V´ertessy, B.G. and Rosta, E.; *J. Am. Chem. Soc.*, **2023**, *145(37)*, 20302–30310.
[3] Csóka, J.; H´egely, B.; Nagy, P.R. and Kállay, M.; *J. Chem. Phys.*, **2024**, *160*, 124113.
[4] Mester, D.; Nagy, P.R., Csóka, J. et al.; *J. Phys. Chem. A*, **2025**, *192(8)*, 2086–2107.

Terahertz spectroscopy of supercritical water – a molecular dynamics approach

Marion Sappl[1,2], Othmar Steinhauser[1], Christian Schröder[1]

[1]University of Vienna, Faculty of Chemistry, Department of Computational Biological Chemistry,
Währinger Str. 17, 1090 Vienna, Austria
[2]University of Vienna, Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria

The critical point of water is at a critical temperature of 647.14 K, a critical pressure of 22.064 MPa and a critical density of 322 kg/m^3 [1]. Above the critical point there is no phase transition between gas and liquid phases. This region is referred to as supercritical fluid. Supercritical water exhibits properties that differ significantly from those of water in its liquid or vapor phases. The terahertz region has only recently been accessible to experimentalists. Therefore, the region between 0.3-10 THz is sometimes referred to as the "terahertz gap". Measuring properties of supercritical water is particularly challenging due to its highly corrosive nature, which necessitates the use of specialized equipment to contain it. Recently, a research group in Bochum successfully determined the terahertz spectrum of supercritical water experimentally and validated their results using *ab initio* molecular dynamics (AIMD) simulations [2].

The AMOEBA multipole force field has previously been shown to reproduce results that closely match experimental data [3]. In this study, we investigated the AMOEBA14 water model in the supercritical region to assess whether the model can accurately describe the terahertz spectrum across a wide range of temperatures and densities. Our findings indicate that the AMOEBA14 water model successfully reproduces the terahertz spectrum for all tested temperatures and densities. Furthermore, we decomposed the spectra into different contributions to identify the origins of spectral changes as water transitions from the liquid to the supercritical phase.

The AMOEBA14 water model utilizes a polarizable multipole force field. In addition to a molecular dipole moment due to point charges, the AMOEBA water model incorporates atomic permanent and induced dipole moments. The spectra can then be separated into permanent and induced contributions. With increasing density, polarization effects decrease and therefore contributions from induced dipoles vanish. The terahertz region is sensitive to both molecular and collective phenomena, making it a unique region where spectra are influenced by the collective molecular dipole moment (including cross-contributions from dipoles interacting with surrounding dipoles) as well as by the fluctuation of molecular dipole moments themselves (self terms). The transition from liquid to supercritical water alters the relative contributions of self-terms and cross-terms to the total spectrum.

Acknowledgments: With partial financial support from the OeAD WTZ grant MK 06/2024.

[1] Levelt Sengers J.M.H.; Straub J.; Watanabe K.; Hill P.G.*J. Phys. Chem. Ref. Data*, **1985**, 14, 193–207.
[2] Mauelshagen K.; Schienbein P.; Kolling I.; Schwaab G.; Marx D.; Havenith M. *Sci. Adv.*, **2025**, 11, eadp8614.
[3] Esser A.; Belsate S.; Marx D.; Head-Gordon T. *Phys. Chem. Chem. Phys.*, **2017**, 19, 5579-5590.

Predicting ligand binding in the age of big data

Jannette Carey

Princeton University, Princeton, NJ, USA

This talk will use four brief historical examples to discuss some constraints inherent to computational prediction of ligand binding that arise from thermodynamics. The discussion will culminate in a challenge to the audience: is it likely that big-data approaches can address this gap? If so, how? What are the pitfalls? If not, what *solvable* problems might stand in the way?

Modeling protein-DNA interactions

Jocelyne Vreede

Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Netherlands

Sequence-specific protein-DNA interactions are central to essential biological processes such as gene regulation and DNA organization. However, experimental investigation of these interactions at high resolution remains challenging. To address this, we present a molecular simulation approach that can quantify the sequence specificity of protein-DNA complexes. By integrating molecular dynamics (MD) simulations with a sophisticated steering potential, our method estimates the free energy difference of protein-DNA dissociation. Applied to the histone-like nucleoid structuring (H-NS) protein, a minor groove binder, the approach accurately predicts nucleotide-specific binding affinities consistent with experimental data and offers mechanistic insights into dissociation pathways. This computational framework enables fast, high-resolution and quantitative prediction of protein-DNA complex stability.

Building on this, we explore the structural basis of H-NS's binding preferences. DNA can have different conformations including A-DNA and B-DNA, depending on hydration or interactions with proteins. H-NS, in particular, shows a strong preference for AT-rich DNA. Employing a combination of spectroscopy and molecular simulation, we were able to demonstrate that H-NS binds ApT-rich sequences with higher affinity than GpC-rich sequences. Upon H-NS binding, AT-rich DNA exhibits increased bending flexibility, minor groove widening, and localized A-like features, while GC-rich DNA retains its canonical B-form. These results reveal how H-NS leverages the intrinsic structural plasticity of DNA to recognize specific sequences, and illustrate the broader principle that DNA-binding proteins can exploit DNA conformational adaptability to fine-tune regulatory functions.

To support these computational and biophysical analyses, we introduce MDNA, a molecular modeling toolkit designed to construct and analyze complex DNA structures. MDNA uses a spline-based mapping technique to generate DNA of arbitrary shape and includes support for canonical and non-canonical base modifications. The toolkit also provides a minimization method for structure refinement and analysis tools based on rigid body formalism. Its modular Python interface streamlines the modeling and analysis of DNA configurations, making it well-suited for integrating into broader molecular simulation workflows.

GRADE-ing Protein-Ligand Interactions

Christian Fellinger[1,2], Thomas Seidel[1,2], Benjamin Merget[3], Christian Schröder[4],
Klaus-Juergen Schleifer[3], Thierry Langer[1,2]

[1]Department of Pharmaceutical Sciences, Faculty of Life Sciences, University of Vienna,
Josef-Holaubek-Platz 2, 1090 Vienna, Austria,
[2]Christian Doppler Laboratory for Molecular informatics in the Biosciences, Department of Pharmaceutical Sciences, University of Vienna, Josef-Holaubek-Platz 2, 1090 Vienna, Austria,
[3]BASF SE, Carl-Bosch-Strasse 38, 67056 Ludwigshafen am Rhein, Germany,
[4]Department of Computational Biological Chemistry, Faculty of Chemistry, University of Vienna,
Währingerstr. 17, 1090 Vienna, Austria

We present **GRADE** [1] (**GR**AIL[2]-based **DE**scriptor), a novel molecular descriptor and machine learning framework for rapid estimation of protein–ligand binding affinities. It targets key outputs such as pKi, pKd, and ΔG. GRADE integrates multiple critical interaction features, including: GRAIL scores from extended pharmacophore modeling via LigandScout [3], Van der Waals interactions, Electrostatic potentials, and Ligand-specific fingerprints independent of receptor structures. These components are combined into a fixed-length vector, optimized for use in predictive modeling.

Our approach, evaluated on both the PDBbind dataset [4] and proprietary industry data, achieves accuracy comparable to leading affinity prediction techniques—while significantly reducing computational cost. The architecture is designed for future integration with GPU acceleration and GRAIL map visualization, further enhancing its applicability to high-throughput virtual screening.

GRADE lays the foundation for a fast, reliable, and scalable structure-based affinity prediction pipeline, with strong potential to accelerate the early stages of drug discovery.

Acknowledgments: The financial support by the Austrian Federal Ministry for Digital and Economic Affairs, the National Foundation for Research, Technology and Development, and the Christian Doppler Research Association are gratefully acknowledged, as well as the financial support and scientific expertise of BASF and Boehringer Ingelheim.

[1] Fellinger, C.; Seidel T.; Merget B.; Schleifer K.-J.; Langer T. *J. Chem. Inf. Model.* **2025**, *65* (5), 2456–2475.
[2] Schuetz D.A.; Seidel T.; Garon A.; Martini R.; Koerbel M.; G. F. Ecker G. F.; Langer T. *J. Chem. Theory Comput.* **2018**, 14 (9), 4958–4970.
[3] Wolber G.; Langer T. *J. Chem. Inf. Model.* **2005**, *45* (1), 160–169.
[4] Su M.; Yang Q.; Du Y.; Feng G.; Liu Z.; Li Y.; Wang R. *J. Chem. Inf. Model.* **2018**, *59* (2), 895–913.

Computational Approaches to Molecular Interactions in Inclusion Complexes of Calix[n]arenes

Khalida Khalil[1,2], Béla Fiser[1,3], Magdalena Małecka[1]

[1] University of Lodz, Faculty of Chemistry, Department of Physical Chemistry,
Pomorska 163/165, 90-236 Lodz, Poland
[2] Doctoral School of Exact and Natural Sciences, Jana Matejki 21/23, 90-237 Lodz, Poland
[3] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary

This study investigates the host–guest interactions between calix[4]arene and a series of organic solvents through a comprehensive computational approach. Key thermodynamic parameters—including interaction energies, enthalpy changes, and Gibbs free energy changes were evaluated alongside geometrical, electronic, and chemical reactivity descriptors to elucidate the effects of molecular encapsulation. All calculations were performed using the B3LYP-D3 hybrid functional with the 6-311+G(d,p) basis set, revealing that the complexes are energetically favorable in both the gas and solvent phases. Notably, the calix[4]arene–DMSO complex exhibits the highest interaction energy (−76.57 kJ/mol) in the gas phase. Frontier molecular orbital (FMO) analysis was conducted to map the distribution of HOMO and LUMO densities, highlighting key electronic features of the complexes. In addition, Interaction Region Indicator (IRI) and Quantum Theory of Atoms in Molecules (QTAIM) analyses were employed to characterize the nature of noncovalent interactions within the systems. The electrophilic and nucleophilic regions of the most stable host–guest complexes were also explored, providing insights into their chemical reactivity and potential applications.

Acknowledgement

We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017769 and PLG/2024/017271.

References:

[1] In Supramolecular Chemistry, Wiley, 2009, pp. 49–104

[2] J.-M. Lehn, Supramolecular Chemistry, Science (80-.)., 1993, 260, 1762–1763

[3] K. Khalil, N. Shahnaz, R. Ludwig, A. M. Tighezza, K. Ayub, T. Mahmood and M. A. Gilani, Unraveling the role of superalkalis in modulating the static and dynamic hyperpolarizabilities of emerging calix[4]arenes, *Phys. Chem. Chem. Phys.*, 2024, **26**, 6794–6805

From genes to machines - multiscale biomolecular simulations

Sarah Harris

School of Mathematical and Physical Sciences, University of Sheffield, Sheffield, S3 7RH, UK

Biomolecular simulations are invaluable for visualising biomolecular dynamics. Here I will give an overview of how we use and develop simulation tools at multiple time and length-scales to understand processes such as molecular recognition, DNA topology and the action of molecular motors. I will highlight the challenges for simulations and how these intersect with experiments, and comment on how these reflect the bigger questions in structural and integrative biology.

Effect of phospholipid headgroups on the membrane penetration of NSO-HET compounds

Zsófia Borbála Rózsa[1], Tamás Horváth[1], Béla Viskolcz[1,2], Milán Szőri[1]

[1] *Institute of Chemistry, University of Miskolc, Egyetemváros A/2, H-3515 Miskolc, Hungary*
[2] *Higher Education and Industrial Cooperation Centre, University of Miskolc, H-3515 Miskolc, Hungary*

Biological membranes, essential to cellular function, are primarily formed by lipid bilayers composed of amphipathic phospholipids. The diversity of the phospholipid headgroups modulates membrane surface charge and intermolecular interactions, shaping key properties such as permeability, mechanical rigidity, and responsiveness to chemical stimuli. Neutral and anionic headgroups — such as choline, ethanolamine, phosphate, and glycerol — contribute to the functional diversity of membranes by altering their electrostatic landscape and lipid packing. [1]

Nitrogen-, sulfur-, or oxygen-containing heterocyclic hydrocarbons (NSO-HETs) are widely used in industrial processes. The presence of their heteroatoms lead to increased water solubility and mobility compared to homocyclic analogues, resulting in persistent environmental contamination and elevated risk to water resources. Due to their lipophilic nature, NSO-HETs primarily target cell membranes, where they can accumulate and disrupt membrane structure and function, as shown previously for 1,4-dioxane, morpholine, and oxane. [2]

To isolate the influence of phospholipid headgroups on the membrane penetration of NSO-HET molecules, model membranes were composed of DPPC, DPPE, DPPA, and DPPG, all sharing identical saturated dipalmitoyl (C16:0) acyl chains, while their headgroups are diverse, containing choline, ethanolamine, a simple phosphorous acid and glycerol respectively. Passive membrane penetration and structural alteration of the membrane structure of representative NSO-HET compounds — 1,4-dioxane, oxane, phenol, and N-methyl-2-pyrrolidone — was examined using molecular dynamics simulations in combination with the adaptive weighted histogram method. [3]

Acknowledgments: We acknowledge the Digital Government Development and Project Management Ltd. for awarding us access to the Komondor HPC facility based in Hungary. We acknowledge the University Research Scholarship Program of the Ministry for Culture and Innovation, funded by the National Research, Development and Innovation Fund.

[1] W. Dowhan, “Molecular Basis For Membrane Phospholipid Diversity: Why Are There So Many Lipids?,” *Annu Rev Biochem*, vol. 66, no. 1, pp. 199–232, Jun. 1997, doi: 10.1146/annurev.biochem.66.1.199.

[2] Z. B. Rózsa, E. Szőri-Dorogházi, B. Viskolcz, and M. Szőri, “Transmembrane penetration mechanism of cyclic pollutants inspected by molecular dynamics and metadynamics: the case of morpholine, phenol, 1,4-dioxane and oxane,” *Physical Chemistry Chemical Physics*, vol. 23, pp. 15338–15351, 2021, doi: 10.1039/D1CP01521D.

[3] V. Lindahl, J. Lidmar, and B. Hess, “Accelerated weight histogram method for exploring free energy landscapes,” *J Chem Phys*, vol. 141, no. 4, p. 044110, Jul. 2014, doi: 10.1063/1.4890371.

Experimental and Computational Insights into Electrospinning Solutions of PVA, Chitosan, and Collagen

Nesreen Alkanakri[1,2], Michael C. Owen [1,2], Babak Minofar[2,3]

[1]Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary.
[2]Higher Education and Industrial Cooperation Centre, University of Miskolc,
3515 Miskolc-Egyetemváros, Hungary.
[3]Department of Physical Chemistry, Faculty of Chemistry University of Lodz,
Pomorska 163/165, Lodz 90-236, Poland.

Nanofibers composed of biopolymers possess incredible potential for biomedical applications [1]. However, poor solubility and structural complexity hinder the electrospinning of natural polymers such as chitosan and collagen [2]. This study integrates electrospinning experiments with Molecular Dynamics (MD) simulations to understand how the molecular structure of the polymers affects their solubility in aqueous environments and, consequently, their ability to form stable nanofibers. Experimental findings confirm that PVA improves the spinnability of chitosan and collagen solutions by enhancing viscosity, preventing phase separation, and facilitating the formation of uniform, defect-free fibers. Increasing the PVA content improves the spinnability of solutions by promoting molecular entanglement within the solution and reducing bead formation. MD simulations of individual PVA, chitosan, and collagen solutions provided molecular-level insights into their solute behavior by revealing that strong intra- and inter-chain interactions in chitosan and collagen promote self-association and hinder dispersion in water. In contrast, PVA exhibited high solubility, chain flexibility, and favorable polymer–solvent interactions, resulting in homogeneous solutions that are consistent with experimental observations. By revealing the molecular interactions that hinder homogeneous solution behavior, this work offers a framework for optimizing electrospinning formulations and improving the processability of structurally complex natural polymers.

Acknowledgments: supported by the EFOP-3.6.1-16-2016-00011 “Younger and Renewing University – Innovative Knowledge City – Institutional development of the University of Miskolc, the National Research, Development and Innovation Office (FK 138501). Calculations were performed at the Komondor supercomputer at the Governmental Agency for IT Development (KIFÜ) in Debrecen.

[1] J. Sharma, M. Lizu, M. Stewart, K. Zygula, Y. Lu, R. Chauhan, X. Yan, Z. Guo, E.K. Wujcik, and S. Wei. *Polymers*. 2015, 7 (2), 186–219.
[2] C. Thambiliyagodage, M. Jayanetti, A. Mendis, G. Ekanayake, H. Liyanaarachchi, and S. Vigneswaran. *Materials*. 2023, 16 (5).

Thermodynamics of Decorporol complexes with Sr^{2+} and Ca^{2+} ions - A combined Isothermal titration Calorimetry and DFT Study

Tamás Horváth[1,2], Zsófia Borbála Rózsa[1], Béla Viskolcz[2], Zoltán Mucsi[1,3,4]
Milán Szőri[1*]

[1] *Institute of Chemistry, University of Miskolc, Egyetemváros A/2, H-3515 Miskolc, Hungary*
[2] *Higher Education and Industrial Cooperation Centre, University of Miskolc, H-3515 Miskolc, Hungary*
[3] *Femtonics Ltd., H-1087 Budapest, Hungary*
[4] *BrainVisionCenter, H-1094 Budapest, Hungary*

E-mail: : tamas.horvath@uni-miskolc.hu

Nuclear incidents release hazardous ^{90}Sr, posing risks to health. Seeking chelating agents capable of removing ^{90}Sr is critical for nuclear safety and development. In our work, the main goal was to develop a substantial, yet straightforward method to support the design of viable, in vivo stable chelating agents for radiostrontium. To investigate, we implemented the highly accurate density functional theory (DFT) based r^2SCAN-3c composite method and isothermal titration calorimetry (ITC). Our methods were validated through the characterization of calcium (Ca^{2+}) and strontium (Sr^{2+}) chelation by ethylenediaminetetraacetic acid (EDTA). The chosen DFT model was able to approximate the literature value ($\Delta\Delta G_{DFT}$ of 15.4 kJ/mol for the ion exchange reaction from Ca-EDTA to Sr-EDTA, compared to the literature value of 11.2 kJ/mol), while the thermodynamic parameters obtained from the ITC study of calcium EDTA chelation are almost identical to those found in the literature. With the validated methods strontium chelation by (7,16-bis-malonate)- 1, 4, 10, 13- tetraoxa- 7,16-diazacyclooctadecane – bis -malonicacid (Decorporol) was examined. Our DFT calculations revealed that the exchange reaction from Ca^{2+} to Sr^{2+} with Decorporol has an exergonic (-14.3 kJ/mol) Gibbs free energy profile, which is also approved by the experimental Gibbs free energy change of -34.5±1.1 kJ/mol obtained from the ITC measurements. Measurements at elevated temperatures and physiological conditions did not impact chelation significantly, therefore in vivo application of the chelating agent is feasible.

Principal Components Modelling of Longitudinal Omics Data

Jeanine Houwing-Duistermaat[1,2], He Li[1], Said el Bouhaddani[3]

[1]*Dept. of Mathematics, Radboud University, 6525AJ, The Netherlands*
[2]*Dept. of Statistics, University of Leeds, LS2 9JT, United Kingdom*
[3]*Dept. of Data Science and Biostatistics, UMC Utrecht, 3584 CX, The Netherlands*

E-mail: Jeanine.duistermaat@ru.nl

Key words: *Latent variable models; Linear mixed models; Dimension reduction; Metabolomics*

For a longitudinally measured omics dataset, the interest might be identifying a set of variables representing the dynamic structure. PCA approaches enable identifying sets of omics variables representing the cross-sectional structure. On the other hand, univariate analysis with fixed and random effects provides insights into whether a variable changes over time but ignores the joint distribution. We propose a novel multivariate dynamic probabilistic PCA-approach (DPPCA) which models the scores over time using a mixed model.

We consider two estimation methods: a two-stage approach and a joint estimation. In the two-stage approach, we first apply PCA to the longitudinal dataset and subsequently fit a linear mixed model to the estimated component scores. In the joint estimation approach, we maximise the log- likelihood using the EM algorithm. Via an extensive simulation study, we evaluate the performance of DPPCA with sample size N=1000 for varying numbers of omics variables (p=5, 100), dynamic components (r=3, 5) and time points (K=3, 5). Finally, we apply DPPCA to a longitudinal metabolomics dataset from the TwinsUK study.

The simulation results show that joint estimation outperforms the two-stage method in estimating the slope (RMSE 0.35 to 0.52 versus 1.00 to 1.45 for first component), whereas the two-stage method performs slightly better in estimating the random intercept variances (RMSE 9.98 to 11.64, versus 7.89 to 8.88). Further, the joint estimation approach shows more robustness when the loading matrices differ. For the 100 metabolites of TwinsUK, a scree plot suggests eight dynamic DPPCA components which explain 75% of the variance. The estimated components appear to change over time and in the first component, most metabolites with high weights are members of the lipoprotein subclasses which are known to change with age. To conclude DPPCA is able to model components changing over time and is also be able to pinpoint relevant features.

Studies on low-barrier $N^{+}–H…O^{-}$ hydrogen bond in pyrimidine – carboxylic acids multicomponent crystals

Agnieszka Rybarczyk-Pirek, Kinga Wzgarda-Raj,
Justyna Dominikowska, Oliwia Bobińska

Department of Physical Chemistry, Faculty of Chemistry, University of Lodz

Hydrogen bonds are especially useful in intermolecular aggregation processes because of their relatively high energy and directionality The enhancement of hydrogen bonding energy by additional factors can lead to a proton transfer phenomenon between formally neutral molecules with the formation of an ionic salt structure according to the scheme: $D–H…A \rightarrow D^{+}–H…A^{-}$. Among various types of hydrogen bonding interactions of special interest are low-barrier hydrogen bonds (LBHB) for which the above process is reversible.

Herein we present results of our researches on cocrystalization of pyrimidines with carboxylic acids. The set of compounds was selected because the carboxyl group is one of the most frequently used functional groups for hydrogen bonding interactions in crystal engineering. In the context of supramolecular chemistry, proton donors (organic acids) and acceptors (pyrimidines - organic bases) are promising agents for generating stable multicomponent hydrogen-bonded systems with potential proton transfer *via* a salt bridge.

The presented studies focus on structural analysis of X-ray diffraction data collected for newly synthesized cocrystals. In particular, the observed supramolecular synthons and stabilizing intermolecular interactions existing in the crystalline state, are analyzed in terms of their directionality, energy and topology. Moreover, the experimental data provide evidence of proton transfer from the carboxylic group to the pyrimidine nitrogen atom, demonstrating the coexistence of neutral and ionic forms of the pyrimidine-carboxylic acid complex, emphasizing tautomeric equilibrium. This phenomenon is further examined with the use of quantum chemical method. The DFT computations are aimed mainly at studying the proton transfer phenomenon but also allow to assess the strength of hydrogen bonds present in the obtained crystal structures.

Acknowledgments: J.D. thanks Prof. Jernej Stare for providing the code for package allowing to solve the one-dimensional time-independent vibrational Schrödinger equation. Calculations were carried out using resources provided by: the Wroclaw Centre for Networking and Supercomputing, grant No. 118; and Polish high-performance computing infrastructure PLGrid (HPC Centre: ACK Cyfronet AGH), grant No. PLG/2024/016984. Access to HPC machines and licensed software is gratefully acknowledged.

New chromone analogues condensed with 1,2,3-triazole as a compounds with potential biological activity

Patryk Czapnik[1,2], Angelika Adamus-Grabicka[3], Małgorzata Domagała[1],
Elżbieta Budzisz[4], Magdalena Małecka[1]

[1]University of Lodz, Faculty of Chemistry, Department of Physical Chemistry,
Pomorska 163/165, 90 – 236 Łódź,
[2]University of Lodz, Doctoral School of Exact and Natural Sciences,
Matejki 21/23, 90 – 237 Łódź,
[3]Medical University of Lodz Faculty of Pharmacy, Department of Medical Chemistry,
Muszyńskiego 1, 90–151 Łódź
[4]Medical University of Lodz Faculty of Pharmacy, Department of Cosmetology,
Muszyńskiego 1, 90 – 151 Łódź

There is a lot of information in the literature about potential biological activity of compounds containing a chromone derivatives and *N*- containing heterocycle ring [1]. There are few reports in the literature on compounds of chromones condensed with 1,2,3-triazoles. Chromone analogues have a lone pair of electrons in the sp^2 hybridized orbital of the azomethine group (Figure 1), which may be crucial for biological activity, especially anticancer potential [2]. On the other hand *N*- heterocyclic compounds are found in commercially available pharmaceutical preparations like tebuconazole or fluconazole [3].

In the present research two chromonocarboxylic acid esters and two chromone analogues with triazoles were synthesized [4]. X-ray crystal structure analysis on all compounds were performed.

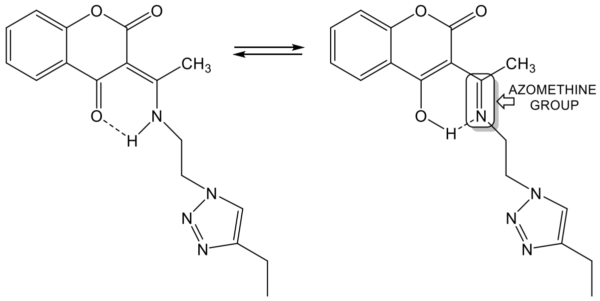


Figure 1. Structural formulas of tautomers of one of the synthesized compounds with marked (frame) the azomethine group responsible for potential biological properties.

In this studies preliminary pharmacokinetic calculations were performed using SwissADME server, which allowed us to determine lipophilicity (log*P*), potential permeability across the blood-brain barrier and the possibility of acting as an inhibitor of certain enzymes [5]. We also carried out preliminary biological studies to evaluate cytotoxic activity on selected cancer cell line: colon (Hct116, LoVo, SW620) and breast (MCF7, MDA-MB0231). The possible toxicity of the obtained compounds and the potential lethal dose value (LD_{50}) were also determined using the ProTox 3.0 program [6].

[1] Abo-Salem, H. et al., *Scientific Reports* **2024**, 14, 1–24.
[2] Boulechfar, C. et al., *Inorganic Chemistry Communications* **2023**, 150, 1–21.
[3] Soujanya, J. et al., *Asian Journal of Chemistry* **2022**, 34 (1), 53–59.
[4] Coppola, G. M., Dodsworth R. W., *Synthesis* **1981**, 7 (1), 523–524.
[5] Daina, A. et al., *Scientific Reports* **2017**, 7, 1–13.
[6] Banerjee, P. et al., *Nucleic Acids Research* **2024**, 52 (W1), W513–W520.

Research towards synthesis of multicomponent crystals consisting of biologically active components

Olga Książkiewicz[1,2], Kinga Wzgarda-Raj[1], Marcin Palusiak[1]

[1] *Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163/165, Lodz, 90-236, Poland,*
[2] *BioMedChem Doctoral School of the University of Lodz and Lodz Institutes of the Polish Academy of Sciences.*

The aim of this research project is to synthesize and characterize new crystalline forms of biologically active compounds using experimental methods. The study focuses on compounds containing cytosine or 4-mercaptopyridine.

Cytosine is a biologically significant molecule, as it is one of the five nucleobases that constitute the genetic code in DNA and RNA. Together with phosphoric acid and sugars, nucleobases form nucleic acids - key biomolecules responsible for the transfer of genetic information and the inheritance of traits in all living organisms [1,2].

In contrast, 4-mercaptopyridine derivatives are organosulfur compounds. 4-mercaptopyridine is a versatile molecule with applications in various fields, including surface chemistry, sensing, and materials science [3]. However, these compounds remain relatively underexplored, with limited literature and few published studies available.

In this work, numerous crystallization experiments were carried out. As a result, five cytosine salts with various carboxylic acids and three co-crystals comprising 4-mercaptopyridine and cyanuric acid were successfully obtained. The resulting crystal structures were determined using single-crystal X-ray diffraction (XRD). Additionally, structural motifs and intermolecular interactions were analyzed.

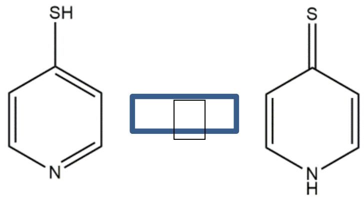


Figure 1: Tautomeric forms of 4-mercaptopyridine.

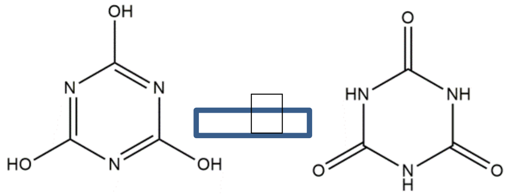


Figure 2: Tautomeric forms of cyanuric acid.

[1] Portalone, G. *Chem. Cent. J.* **2011**, *5*, 51
[2] Książkiewicz, O. *Acta Cryst. C* **2024**, *C80*, 742-747
[3] Guo, H.; Ding, L.; Mo, Y. *J. Mol. Struct*. **2011**,*991*, 103-107

ATP-peptide interactions And Peptide Aggregation

Dominik Horinek

Institute of Physical Chemistry, University of Regensburg, 93053 Regensburg, Germany

Recently, it was experimentally shown that the solubility of proteins in water can be enhanced by the addition of adenosine triphosphate (ATP) [1]. To investigate the underlying molecular interactions, we performed molecular dynamics (MD) simulations of ATP and homopeptide chains composed of glycine, tryptophan, lysinium and glutamate [2]. The potential of mean force (PMF) as a function of the ATP-peptide distance was calculated using umbrella sampling with a self-developed force field [3]. Splitting of the interaction energy into a van der Waals and a Coulomb contribution gives further insight into the mechanism of the solubility enhancement. The analysis reveals that ATP is attracted to all studied proteins. This suggests that the enhancement of the protein solubility might stem from the affinity of ATP to the protein surface. We further studied the effect of ATP on amyloid aggregation using advanced free-energy methods [4]. Decomposition of the free energies reveals that van der Waals interactions with the peptide are decisive in determining the relative stabilization of the monomeric state.

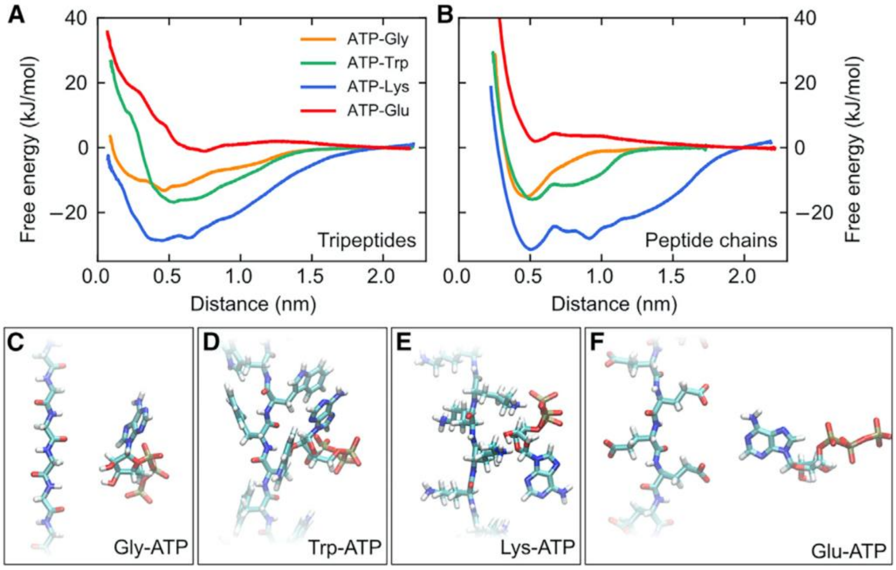


Figure 1. *Protein-ATP interaction free energies for different polypeptides.*

References

[1] A. Patel, L. Malinovska, S. Saha, J. Wang, S. Alberti, Y. Krishnan and A. A. Hyman, ATP as a biological hydrotrope, Science, 356, 753–756 (2017).

[2] J. Mehringer, T.-M. Do, D. Touraud, M. Hohenschutz, A. Khoshsima, D. Horinek and W. Kunz, Hofmeister vs. Neuberg – Is ATP really a biological hydrotrope?, Cell Rep. Phys. Sci., 2, 100343 (2021).

[3] T.-M. Do, N. Matubayasi, D. Horinek, Development of a force field for ATP – how charge scaling controls self-association, Phys. Chem. Chem. Phys. 27, 6325 (2025).

[4] T.-M. Do, D. Horinek, N. Matubayasi, How ATP suppresses the fibrillation of amyloid peptides: analysis of the free-energy contributions, Phys. Chem. Chem. Phys. 26, 11880 (2024).

Interactions in models of Thioredoxin reductase; DFT & QM/MM studies

Jaroslav V. Burda[1], Adam Vavrečka[1], and Milan Říha[2]

[1]*Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Prague, 12116, Czech Republic*
[2]*Department of Chemistry, Faculty of Science, Masaryk University, Brno, 62500, Czech Republic*

Oncological diseases can be also cured with programmed cell death (PCD) induced by increased oxidative stress. One of the main PCD types is so-called apoptosis, which is regulated by thioredoxin systems. [1] The thioredoxin reductase enzyme, one of the key thioredoxin system components, can be blocked by gold(I) complexes and hence cause therapeutic oxidative stress. [2]

First, we investigated the interactions of a selected gold(I) complex with the active site of the enzyme using the density functional method. For this purpose, structures of reactants, transition states, and products in different redox states and (de)protonations of the active site were explored. We started from simple model where gold(I)-NHC complex interacts with amino acid (Cys or Sec). From these calculations, pH dependence of Gibbs-Alberty activation energies and reaction energies from the reaction profiles were determined.[3]

Recently QM/MM MD calculations were performed using Umbrella sampling technique on the several systems where the quantum core comprised water[4], isolated amino acids (Cysteine and/or Selenocysteine, and terminal tetrapeptide sequence from the C-end of the enzyme together with the gold(I)-NHC complex in explicit water solvation box based on TIP3P empirical potential for mimicking aqua solution. These systems were compared with previous quantum chemical calculations within implicit solvent models. The differences and other properties will be discussed.

All the computational models predict spontaneous gold coordination to both S- and Se-sites especially in neutral and basic environments.

References:

[1] Lu, J.; Holmgren, A. Thioredoxin System in Cell Death Progression. *Antioxidants & Redox Signaling* **2012**, 17 (12), 1738-1747.

[2] Rubbiani, R.; Kitanovic, I.; Alborzinia, H.; Can, S.; Kitanovic, A.; Onambele, L. A.; Stefanopoulou, M.; Geldmacher, Y.; Sheldrick, W. S.; Wolber, G.; Prokop, A.; Woelfl, S.; Ott, I., Benzimidazol-2-ylidene Gold(I) Complexes Are Thioredoxin Reductase Inhibitors with Multiple Antitumor Properties. *J. Med. Chem.* **2010**, 53, 8608–8618.

[3]. Říha, M.; Muzarová M.; Burda, J.V: J. Phys. Chem. pH control of the reaction mechanism: interactions of the Au(I)-NHC complex with thioredoxin reductase (modeled by cysteine and selenocysteine); ab initio and DFT calculations. Phys. Chem. Chem. Phys., 2025, 27, 6604–6615.

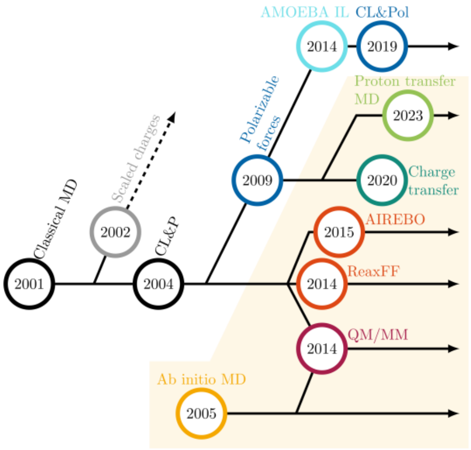
[4]. Říha, M.; Munzarova, M.; Burda, J.V. Gold(I)–N–heterocyclic carbene hydration process; ab initio , DFT, and QM/MM molecular dynamics study. J. Chem. Phys. 162, 214301 (2025);

Advancing Proton Transfer Simulations in Ionic Liquids

Márta Gődény, Florian Joerg, Christian Schröder

University of Vienna, Faculty of Chemistry, Department of Computational Biological Chemistry

Proton transfer reactions in protic ionic liquids play a pivotal role in determining macroscopic properties such as conductivity, viscosity, and chemical reactivity [1]. Modeling these reactions at the molecular level remains challenging due to the complex interplay of hydrogen bonding, solvation structure, and dynamic proton hopping mechanisms. The Python-based PROTEX framework [2] addresses these challenges by enabling reactive MD simulations with polarizable force fields. Originally designed for neat protic ionic liquids, PROTEX has now been significantly expanded to support a broader range of systems [3], including photoacids and molecular solvents like methanol.



Overview of MD simulation on ionic liquids [1]

Unlike continuous reactive force fields, such as ReaxFF or AIREBO, PROTEX efficiently supports large-scale simulations with hundreds of simultaneous proton transfer by maintaining a fixed molecular topology and intermittently updating atomic identities based on predefined reaction schemes. This enables the exploration of phenomena such as proton conductivity and charge transport across experimentally relevant time and length scales, scenarios where quantum and multiscale methods remain computationally prohibitive. Also, the latter methods do not necessarily reproduce the experimental composition of the molecules involved in the reaction. In PROTEX, the composition of the molecules can be enforced to stay as close as possible to the experiment. Also, charge transfer reactions can be modelled by PROTEX.

[1] Gődény, M., Schröder, C., *Liquids* 2025, 5, 8.
[2] Joerg, F., Wieder, M. Schröder, C., *Front. Chem.: Molecular Liquids* 2023, 11, 1140896
[3] Gődény, M., Joerg F., Kovar, M. P.-P., Schröder C., *J. Phys. Chem. B* 2024, 128, 3416

Atomistic Simulations for Sustainable Chemistry and Environmental Safety: From Chlorine Storage to PFAS–Plastic Interactions

Milán Szőri

Institute of Chemistry, University of Miskolc, Egyetemváros A/2, H-3515 Miskolc, Hungary

In this presentation, recent advancements in the integration of molecular simulations with experimental techniques are discussed, aimed at addressing two critical challenges in industrial and environmental chemistry: the safe storage of chlorine and the environmental fate of perfluoroalkyl substances (PFASs).

In the first part, classical molecular dynamics (MD) simulations are employed to investigate the storage and release mechanisms of molecular chlorine in triethylmethylammonium chloride-based ionic liquids. These systems are identified as promising candidates for safe and reversible chlorine carriers due to their high storage capacity and thermal stability, thereby addressing key vulnerabilities in the global chlorine supply chain.

In the second part, the aquatic environmental behavior of emerging contaminants is explored through a combination of experimental (electrophoretic and dynamic light scattering) and computational (MD) methods. Specifically, the adsorption mechanism of undecafluorohexanoic acid (UFHA), a short-chain PFAS, onto charged polystyrene microplastic surfaces is examined. The results indicate a strong, salt-independent interaction between the charged functional groups of PFASs and polystyrene, mediated by hydrogen bonding and resulting in charge inversion and aggregation near the isoelectric point.

These findings provide molecular-level insights that inform the development of safer chemical storage solutions and enhance our understanding of pollutant behavior in aqueous environments. The work underscores the synergistic potential of combining molecular simulations with experimental approaches in advancing sustainable chemistry.

Making and breaking polyurethanes

György Marcell Tokaji[1,2], Anikó Csábrádiné Jordán[3], Rehana Bano[1,3], Péter Tóth[2], László Farkas[2], Béla Viskolcz[1,3], Emma Szőri-Dorogházi[1], Milán Szőri[1], Zsanett Renáta Boros[2], Béla Fiser[1,4]

[1]Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary,
[2]Wanhua-BorsodChem Zrt, Bolyai tér 1., H-3700 Kazincbarcika, Hungary,
[3]Higher Education and Industrial Cooperation Centre, University of Miskolc,
3515 Miskolc-Egyetemváros, Hungary,
[4]Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland

Polyurethanes (PUs) are versatile polymers widely used in insulation, coatings, adhesives, foams, and elastomers due to their tunable mechanical and chemical properties. However, their increasing global production and limited recyclability pose significant environmental challenges, highlighting the need for deeper mechanistic understanding and recycling strategies.

Chemical and biodegradation of PU was studied by using various techniques including theoretical and experimental approaches. A model system for urethane chemistry was developed through the synthesis of a diurethane compound from 2,4-toluene diisocyanate (2,4-TDI) and 1-butanol in acetonitrile, under both catalyst-free and DABCO-catalyzed conditions. Optimal reaction parameters were established to obtain a pure and reproducible diurethane product. The reaction pathways were also described by computational chemistry tools. The degradation of the model system was described and preliminary results demonstrated that TDI-based urethanes have a potential for easier separation and recovery of valuable chemical fractions, offering promising ways for recycling of polyurethane wastes.

Acknowledgments: Financial support by the National Research, Development and Innovation Fund (Hungary) within the TKP2021-NVA-14 project and the Co-Operative Doctoral Program of the Ministry of Innovation and Technology was provided.

Biosorption and Bioaccumulation of Nickel by Chlorella vulgaris

Peter Koska[3], Timea Fóris[3], Kitty Gráczer[1], Bela Fiser[1,2], László Vanyorek[1],
Béla Viskolcz[1,3]

[1] *Institute of Chemistry, University of Miskolc, Miskolc-Egyetemváros, 3515 Miskolc, Hungary.*
[2] *Department of Physical Chemistry; Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland,*
[3]*Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc, Hungary*

In recent study biosorption and bioaccumulation of nickel were studied with Chlorella vulgaris microalga. In the case of biosorption studies kinetics of nickel absorption, and efficiency of adsorption was studied as a function of initial nickel concentrations and cell concentrations. Our new finding was that the adsorbed nickel increases logarithmically as a function of the initial nickel concentrations, and the algal surface becomes saturated with nickel ions around initial nickel concentration of 40mg/L. The specific adsorption rate of nickel decreased exponentially by the increase of cell concentration (Figure1.).

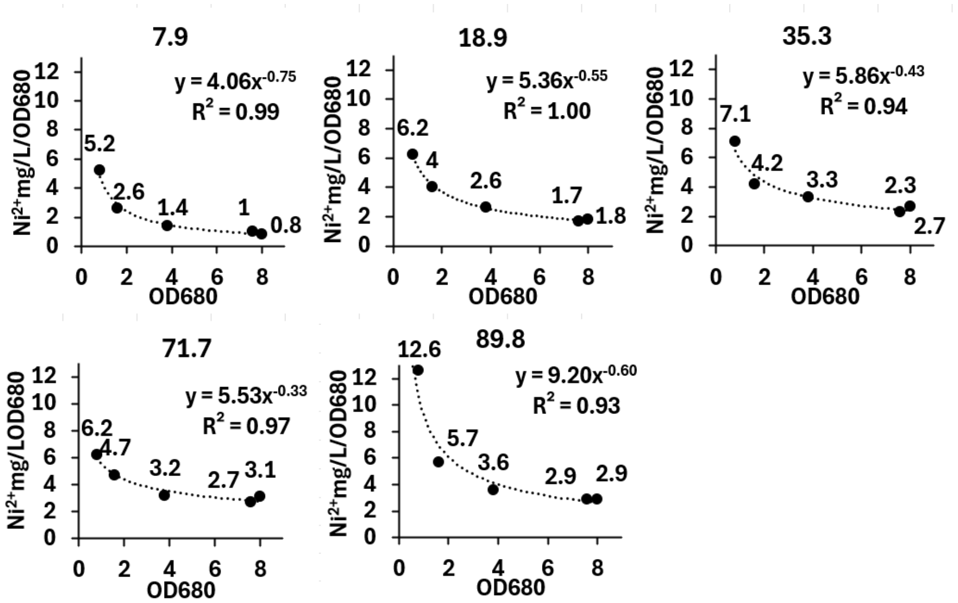


Figure1. Specific adsorption rate of nickel as a function of cell concentration expressed in OD680 value on “x” axis. The numbers in the title row of the plots mean the initial nickel concentration expressed in mg/L

In the case of bioaccumulation, we detected nearly total removal of nickel by the 48. hour of incubation time in potassium-nitrate containing medium. Nickel removal efficiency was more than 90% at 24., and 48. hours of incubation when di-ammonium-phosphate was applied as nitrogen source. In summary nickel removal with bioaccumulation can be more efficient than in the case of biosorption which is impaired by the decreasing specific adsorption by increasing cell concentration.

Computational and Experimental Study of Antioxidant Polymer Additives

Dalal K. Thbayh[1,2,3, *,] Béla Fiser[1,3,4,5**]

[1]Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary
[2]Polymer Research Center, University of Basrah, Basrah, Iraq
[3]Higher Education and Industrial Cooperation Centre, University of Miskolc,
3515 Miskolc-Egyetemváros, Hungary
[4]Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland
[5]Ferenc Rakoczi II Transcarpathian Hungarian College of Higher Education,
90200 Beregszász, Transcarpathia, Ukraine

e-mail: *dalal.thebayh@uobasrah.edu.iq ** bela.fiser@uni-miskolc.hu

Antioxidant additives and stabilizers are chemical substances frequently employed in many industries, such as food and polymer processing. Despite their distinct goals, we can identify some convergence in their functions, particularly in the realm of polymers and specific materials [1]. One thing they all have in common is that antioxidants can act as stabilizers, particularly when preventing oxidation-induced degradation. In polymers and plastics antioxidants are frequently used to prevent or slow down polymer degradation due to oxidation processes. In this sense, antioxidants are a type of stabilizer that specifically addresses the oxidative degradation of materials. Thus, they aid in the preservation of the material's physical and mechanical qualities throughout time. Furthermore, some stabilizers may have antioxidant properties, and some antioxidants may offer stability against factors beyond oxidation. The specific requirements of the material and the conditions it will encounter determine the choice of additives. For instance, heat, oxidative conditions, and ultraviolet radiation may require stabilizers and antioxidants for a plastic material like PVC to ensure long-term stability.

[1] Dalal K. Thbayh, and Béla Fiser, *Polym. Degrad. Stab*, 201 (2022): 109979.

Biological removal of heavy metals from water

Tímea Fóris[1], Péter Kóska[2], László Vanyorek[1], Béla Viskolcz[1,2]

[1] *Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary*
[2] *Higher Education and Industrial Cooperation Centre, University of Miskolc,*
3515 Miskolc-Egyetemváros, Hungary

Algae, encompassing both microalgae and macroalgae, represent a highly promising and sustainable solution for the remediation of heavy metal contamination in aquatic environments. Their unique biological and physiochemical properties enable efficient binding and removal of various toxic metal ions, offering a compelling alternative to conventional, often costly and less environmentally friendly, methods.

Algae employ a sophisticated array of strategies to bind heavy metal ions. In the first part of the presentation, I will introduce the measurement methods we used to examine the metal binding of algae. We found biosorption to be the dominant process, while the role of bioaccumulation was negligible in our experiments.

Next, we will attempt to show how algae "covered" with heavy metals can be removed using magnetic nanoparticles. Beyond analyzing the interactions between cobalt. nanoparticle and algae, we will also demonstrate the industrial applications of this method. [1]

We involved high school students in the experiments as part of a one-year extracurricular activity. In this project, it was important for the students to independently gather information on a scientific topic, design the experiment, analyse the data and draw conclusions from the processed data.

Acknowledgments: This research was supported by the National Research, Development, and Innovation Fund (Hungary), within the TKP2021-NVA-14 project. Financial support for the creation and complex development of National Laboratories within the RRF-2.3.1-21-2022-00014 Climate Change Multidisciplinary National Laboratory project is also acknowledged.

[1] Fóris, T.; Koska, P.; Ilosvai, Á.M.; Kristály, F.; Daróczi, L.; Vanyorek, L.; Viskolcz, B. *Int. J. Mol. Sci.* **2025**, *26*, 5467. https://doi.org/10.3390/ijms26125467

Designing the Future of Photonics: Superalkali Based Electrides and Alkalides for Enhanced Nonlinear Optical Response

Rehana Bano [1,2*], Béla Viskolcz[1,2], Béla Fiser[1,3,]

[1] *Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary*
[2] *Higher Education and Industrial Cooperation Centre, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary*
[3] *Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland*

The fabrication of stable nonlinear optical (NLO) materials is essential due to their growing applications in optoelectronics. Several complexes showing high nonlinear optical response (NLO) have been reported both theoretically and experimentally. More recently, a special kind of compounds containing diffuse excess electrons has been designed that considerably enhances the NLO response of various organic and inorganic systems. Recently, superalkali-based compounds with diffuse excess electrons have emerged as promising candidates to significantly enhance NLO properties. Novel NLO materials were designed using DFT simulations, including superalkali electrides and alkalides, mixed superalkali electrides, and alkaline earth metal-based alkalides. Comprehensive analyses (NBO, MEP, NCI, QTAIM, and TD-DFT) were performed to study their geometry, stability, electronic structure, and NLO behavior. Li_2F and Li_3F superalkali-doped $Al_{12}N_{12}$ electrides (A–E) demonstrated strong interaction energies (-52.97 to -87.58 kcal/mol) and significantly reduced HOMO-LUMO gaps (5.44-5.87 eV), resulting in enhanced NLO responses, with maximum first and second hyperpolarizabilities reaching 1.20×10^{4} and 1.65×10^{4} au, respectively. High nonlinear refractive indices (up to 5.41×10^{-11} cm^2/W) were also achieved [1]. Similarly, mixed superalkali clusters doped with $B_{12}N_{12}$ showed even higher stability (interaction energies up to -123.13 kcal/mol) and smaller HOMO-LUMO gaps (3.36–4.27 eV). These complexes exhibited strong NLO activity with a maximum first hyperpolarizability of 1.7×10^{7} au and transparency in the UV region with absorption in the NIR (1076–1486 nm) [2]. Furthermore, novel Janus-type alkaline earthide complexes M_3O^--1-M' (M = Li, Na, K; M' = Be, Mg, Ca) also showed remarkable NLO performance with enhanced hyperpolarizabilities and strong SHG, EOPE, and HRS responses. The maximum quadratic nonlinear refractive index reached 2.16×10^{-7} cm^2/W. These findings offer a valuable pathway for the design of next-generation, high-performance NLO materials suitable for advanced optoelectronic applications.

Keywords: Electrides; Alkalides; Nonlinear optical materials; DFT; Experimental

Acknowledgments: This research was supported by the National Research, Development and Innovation Fund (Hungary) within the TKP2021-NVA-14 project.

References:

[1] Bano, R.; Arshad, M.; Mahmood, T.; Ayub, K.; Sharif, A.; Tabassum, S.; Gilani, M. A. Superalkali (Li2F, Li3F) Doped Al12N12 Electrides with Enhanced Static, Dynamic Nonlinear Optical Responses and Refractive Indices. *Mater. Sci. Semicond. Process.* **2022**, *143*, 106518. https://doi.org/10.1016/j.mssp.2022.106518.

[2] Bano, R.; Ayub, K.; Mahmood, T.; Arshad, M.; Sharif, A.; Tabassum, S.; Gilani, M. A. Mixed Superalkalis Are a Better Choice than Pure. *Dalt. Trans.* **2022**, *51*, 8437–8453. https://doi.org/10.1039/d2dt00321j.

Ecotoxicological Assessment of Polyurethane Foams and Bio-Based carbonaceous Materials: Environmental Impacts and Applications

Julie Mallouhi[1,2], Emőke Sikora[1,2], Kitti Gráczer[1], Olivér Bánhidi[1], Sarra Gaspard[3], Francesca Goudou[3], Béla Viskolcz[1,2], Emma Szőri-Dorogházi[1,2,*], Béla Fiser[1,2,4,5,*]

[1]*Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary*
[2]*Higher Education and Industrial Cooperation Centre, University of Miskolc,*
3515 Miskolc-Egyetemváros, Hungary
[3]*Laboratory COVACHIM-M2E, EA 3592 Université des Antilles,*
BP 250, 97157Pointe à Pitre Cedex, Guadeloupe
[4]*Ferenc Rakoczi II Transcarpathian Hungarian College of Higher Education,*
90200 Beregszász, Transcarpathia, Ukraine
[5] *Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland*

E-mail: julie.mallouhi@gmail.com

Polyurethanes (PUs) are widely used polymers that differ from conventional polymers. However, they often end up in landfills, releasing toxic compounds when degraded by environmental or human factors [1]. In this study, toxicity test protocols were developed by using *Sinapis alba* seeds and two bacteria (*E. coli* and *M. luteus*) to assess five PU foam samples with varying NCO indices and compared to the Control sample. Results showed that the higher toxicity was observed in the case of samples with higher NCO indices (especially NCO-1.2) compared to the Control sample. In the bacterial test, it was observed that the samples containing NCO-1.1 and NCO-1.2 had lower colony numbers (5.0×10^8 and 4.9×10^8 CFU/mL, respectively). All in all, two toxicity tests were successfully adapted for PU foams, and both are applicable in the ecotoxicological assessment of the samples. These protocols were also applied to carbonaceous materials derived from natural sources, including activated carbon (AC) and biochar (BC) from *Sargassum sp.*, and compared to commercial AC [2]. All showed no toxicity, suggesting their potential for environmental applications. Therefore, these non-toxic bio-based carbonaceous materials were used as adsorbents to remove cobalt ions from water. Adsorption tests were conducted to assess the capacity of AC and BC to remove cobalt ions from water. The results showed that the AC derived from *Sargassum* sp. has the highest adsorption capacity due to the high surface area, which offers more active sites for interactions with adsorbates.

Keywords: Polyurethane foam, Toxicity tests, Activated carbon, Biochar, *Sargassum* sp. Adsorption of Co ions.

Acknowledgments: Financial support has been provided by the National Research, development, and Innovation Fund (Hungary) within the TKP2021-NVA14 project.

[1] N.R. Gunawan, M. Tessman, A.C. Schreiman, R. Simkovsky, A.A. Samoylov, N.K. Neelakantan, T.A. Bemis, M.D. Burkart, R.S. Pomeroy, S.P. Mayfield. *Bioresour Technol Rep*. **2020**, *11*.

[2] R. Ranguin, M. Delannoy, C. Yacou, C. Jean-Marius, C. Feidt, G. Rychen, S. Gaspard. *J Environ Chem Eng*. **2021**, *9*.

Abstracts of poster presentations

Symmetric O···H···O and asymmetric O–H···O hydrogen bonds in multicomponent crystals of pyridinedicarboxylic acids

Anna Ben[1,2], Justyna Dominikowska,[1] Béla Fiser,[1] Lilianna Chęcińska[1]

[1]*Faculty of Chemistry, University of Lodz, Pomorska 163/165, 90-236 Lodz, Poland*
[2]*University of Lodz Doctoral School of Exact and Natural Sciences, Narutowicza 68, 901-136 Lodz, Poland*

Crystal engineering has a wide range of applications in many fields, enabling modification and control of material properties through cocrystallization. This technique uses repeating structural motifs created by intermolecular interactions between functional groups of molecules to design new crystals. Understanding molecular assembly in nature is crucial to creation of multicomponent crystals with predictable structures and desired properties. Crystal engineering is particularly effective in developing pharmaceutical cocrystals and salts [1].

In our projects, we combined the idea of crystal engineering with the potential of pyridinedicarboxylic acids to create a remarkable variety of supramolecular frameworks. We cocrystallized isomeric pyridine-2,*n*-dicarboxylic acids (*n*=3,4,5,6) with miconazole [2] and enrofloxacin [3]. This led to formation of new salts that were characterized by single-crystal X-ray diffraction. Interestingly, acid molecules were found to be responsible for the formation of unique polymeric chain motifs and common mono-periodic supramolecular chains, driven by symmetric O···H···O and asymmetric O−H···O hydrogen bonds, respectively. The analysis of these interactions using the quantum theory of atoms in molecules revealed significant differences in their properties. Additionally, density functional theory calculations were employed to investigate proton transfer in molecular pairs present in polymeric chains, offering deeper insight into the formation of symmetric interactions in the solid state.

[1] Desiraju, G. R. In Crystal Engineering: The Design of Organic Solids. **1989**, Elsevier, Amsterdam.
[2] Ben, A.; Dominikowska, J.; Fiser, B.; Chęcińska, L. *Cryst. Growth Des.*, **2025**, doi: 10.1021/acs.cgd.5c00239.
[3] Hushcha, V.; Ben, A.; Felczak, A.; Lisowska, K.; Kinart, Z.; Gacki, M.; Chęcińska, L. *Scientific Reports*, **2024**, *14*, 29317.

New polymorph of methyl 3,4-dicyano-1-methyl-2,5-diphenylpyrrolidine-3-carboxylate

Małgorzata Domagała

Faculty of Chemistry, University of Lodz, 90-236 Lodz, Pomorska 163/165, Poland

Two polymorphs of methyl 3,4-dicyano-1-methyl-2,5-diphenylpyrrolidine-3-carboxylate were obtained in the recrystallization process using two different solvent mixtures. The structure I, from petroleum ether/methylene chloride, crystallized in orthorhombic crystal system in $Pna2_1$ space group, while structure II [1], from ethanol/methylene chloride, crystallized in monoclinic system in $P2_1/c$ space group.

The crystallographic calculations and comparative analysis of the geometry of both structures show the clear difference in molecules organization and the formation of intra- and intermolecular interactions. A small differences in the geometry of molecule in both structures and a large difference in crystal packing, suggest a packing polymorphism. The Hirshfeld surfaces analysis and the "fingerprint plots" analysis confirmed this thesis.

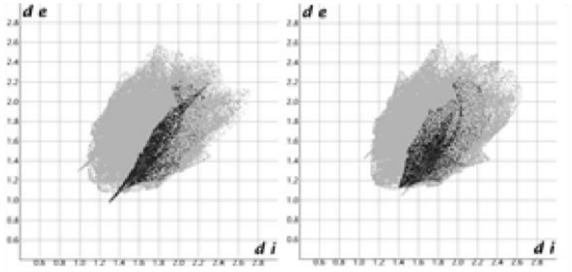


Figure 1: Fingerprint plots for O…H interactions existing in the crystal structures of both polymorphs, $Pna2_1$ (left) and $P2_1/c$ (right)

Moreover, for both structures of the title compound the periodic calculations in Crystal09 were performed. The formation energy of a molecular crystal, obtained as a difference between the energy of the bulk and the sum of the energies of isolated molecules, differs by about 3 kcal/mol only.

Acknowledgments: M.D. acknowledges the Wroclaw Centre for Networking and Supercomputing (http://www.wcss.pl) and PLGrid Infrastructure (PLG/2025/018176) for providing access to HPC machines and licensed software.

[1] Mlostoń, G.; Urbaniak, K.; Domagała, M.; Pfitzner, A.; Zabel M. and Heimgartner, H. *Helv. Chim. Acta*, **2009**, *92*, 2631-2642.

Plasmon-Enhanced Fluorescence Analysis of DNA Origami Immobilized on Gold Nanoparticles

Tímea Gerzsenyi[1], Duncan Sutherland[2]

[1] Higher Education and Industrial Cooperation Center, University of Miskolc, Miskolc 3515, Hungary
[2] Interdisciplinary Nanoscience Center, Aarhus University, Aarhus C 8000, Denmark

Biological materials in living systems assemble in a bottom-up manner, guided by the molecular information encoded within biomolecules. This intrinsic programming drives not only self-assembly but also the hierarchical organization of increasingly complex structures, achieving near-atomic precision across length scales from the nanometer to the macroscopic. In contrast, in vitro fabrication of 3D nanostructures has generally lacked comparable precision and controllability. In the present study, we investigated the assembly of single-stranded DNA molecules immobilized on gold nanoparticle surfaces to form DNA origami structures. The hybridization of complementary DNA strands was facilitated using a freeze–thaw annealing method. We evaluated the binding efficiency of complementary strands introduced at various time points to functionalized nanoparticles. The final structural component was a short, fluorophore-labeled ssDNA comprising only a few nucleotides. The transient binding events of this labelled strand were monitored using total internal reflection fluorescence (TIRF) microscopy. Gold nanoparticles played a significant role due to their localized surface plasmon resonance (LSPR), which significantly enhanced the fluorescent signal (plasmons-enhanced fluorescence) enabling single-molecule resolution in the detection of DNA binding events on individual particles. The effect was further examined using different nanoparticle coatings (citrate, CTAB). Data analysis was conducted using *Plasmon* software in conjunction with custom MATLAB scripts. This approach holds promise for biosensor development, especially for detecting specific DNA sequences in diagnostic platforms. It also enables real-time analysis molecular interactions, including drug-target binding events. Building on this foundation, we also engineered a composite biomolecular origami structure incorporating DNA, carbohydrate ligands, and a fluorescently labelled protein. Two types of glycans — monovalent and trivalent — were employed to probe differences in multivalent binding interactions with the associated protein target. This work establishes a versatile platform for the study of molecular recognition, with potential implications for drug delivery, diagnostics, and nanotherapeutics.

Multifunctional Polyurethane Foams: Influence of Ag_2O Doping on Structural and Functional Properties

Adnan M. Khan[1], Marcell D. Csécsi[1], Dóra Mentes[1,2], László Farkas[2],
Béla Fiser[1,2,3], Béla Viskolcz[1,2]

[1] Institute of Chemistry, University of Miskolc, 3515 Miskolc-Egyetemváros, Hungary
[2] Higher Education and Industrial Cooperation Centre, University of Miskolc,
3515 Miskolc-Egyetemváros, Hungary
[3]Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, 90-236 Lodz, Poland

The development of multifunctional lightweight materials is critical for modern engineering applications requiring combined mechanical strength, thermal stability and sound absorption. We investigate the fabrication and characterization of polyurethane foams (PUFs) doped with varying concentrations of silver oxide (Ag_2O) to enhance their overall performance. PUFs were synthesized with Ag_2O contents of 1%, 5%, 10%, 50%, 75% and 100% by weight. A comprehensive set of tests including ammonia soaking tests, compression testing, thermal degradation analysis and acoustic absorption measurements employed to evaluate the distributional, structural and functional characteristics of the resulting hybrid foams.

Ammonia soaking tests indicated uneven distribution of Ag_2O particles, with frequent accumulation on the pore surfaces. This was attributed to inadequate dispersion during mixing and suboptimal compatibility between the inorganic filler and the polymer matrix. Despite this, a positive correlation was observed between Ag_2O concentration and compressive strength, with the 100% Ag_2O-doped foam exhibiting the highest resistance to deformation under load.

Acoustic performance, however, showed a non-linear trend. The foam doped with 10% Ag_2O demonstrated the best acoustic absorption behaviour, achieving an absorption coefficient greater than 0.95 in the critical 3000–5000 Hz frequency range. Higher doping levels ($\geq$50%) resulted in diminished acoustic and thermal performance, likely due to agglomeration of Ag_2O particles and decreased pore interconnectivity, which hindered effective sound wave dissipation and thermal insulation.

These findings suggest that a 10% Ag_2O concentration offers the most favourable balance between mechanical reinforcement and acoustic efficiency. This optimized hybrid foam presents strong potential for use in applications such as noise-dampening panels, lightweight insulation materials and multifunctional structural components in the automotive and construction sectors.

Acknowledgments: This research is supported by the National Research, Development, and Innovation Fund (Hungary) within the TKP2021-NVA-14 project. This work has been implemented by the National Multidisciplinary Laboratory for Climate Change (RRF-2.3.1-21-2022-00014) project within the framework of Hungary's National Recovery and Resilience Plan supported by the Recovery and Resilience Facility of the European Union.

[1] Szycher, M. Structure–Property Relations in Polyurethanes. In *Szycher's Handbook of Polyurethanes, Second Edition*; CRC Press, 2012; pp 37–86. https://doi.org/10.1201/b12343-4.

Computational Characterization of LPS Membranes and Their Interaction with Alternariol

Nuša Matjašec

University of Vienna, Faculty of Chemistry, Währinger Str. 17, 1090 Vienna, Austria

Urinary tract infections are among the most common bacterial infections, primarily caused by Gram-negative bacteria as *Escherichia coli*. Their outer membrane is rich of lipopolysaccharides (LPS), which are known to induce an immune response through the binding to the TLR receptors on the bladder epithelium. Other surface receptors, such as integrins, also appear to play an important role in modulating the inflammatory response, as they support cell adhesion and maintain tissue integrity. Additionally, the presence of dietary xenobiotics with immunomodulatory potential, as alternariol (AOH), may affect the interactions between proteins and LPS or alter cell morphology of the bladder cells. To gain a better understanding of the molecular pathomechanisms involved in bladder infections, molecular dynamics simulations were used to build and analyze systems of LPS membranes with β1 integrins and dietary xenobiotics. First, a simplified system of a LPS bilayer was generated using CHARMM-GUI. To study the influence of calcium ions on the membrane stability, two systems of the membrane were generated and combined with 10 AOH molecules using CHARMM. The simulations were performed with OpenMM and were analyzed with MDAnalysis. Whereas the water distribution in the two different systems was comparable, our simulations showed that in the system containing calcium ions, Alternariol was mainly distributed in the oligosaccharide region of the membrane. Neither of the systems showed any disruption or destabilization the core lipid structure. In the next step, LPS membrane simulations were carried out with β1 integrins. The aim is to get a deeper understanding of the chemical and microbe interactions within the bladder and provide essential insights for targeted drug development.

Overview of potassium channel selectivity filter occupancy by K^+ ions and water molecules

Milan Melicherčík[1], Ivan Kĺbik[2], Ivan Sukuba[1], Pavel Mach[1]

[1] Department of nuclear physics and biophysics, Faculty of Mathematics, Physics and Informatics,
Comenius University in Bratislava, Michala Greguša 1, 842 48 Bratislava, Slovakia;
[2]Institude of Physics SAS, Dúbravská cesta 9, 845 11 Bratislava, Slovakia

Potassium channels are transmembrane proteins composed of four identical monomers. The selectivity filter is formed by a five residue sequence, TVGYG (or TIGYG in some eukaryotic cells), within each of the four subunits in transmembrane part. Selectivity filter is very conserved part of all potassium channel and filters only K^+ ions. Even Nobel price was awarded in 2003 for explaining its filtering capabilities, there are sill some controversy about its function.

The selectivity filter has 4 internal positions for ions, clearly visible on some crystal structures from high concentration K^+ solutions (e.g. KcsA channel PDB code: 1K4C, claimed to be in conductive state). There exists another opinion based on MD simulations with classical force fields, IR spectroscopy and mutant X-ray structures (mutated residues were directly in selectivity filter) claiming water molecules alternates K^+ ions in channel (K^+-water-K^+-water or water-K^+-water-K^+ configurations) – for more information and references see e. g. [1]

Classical MD simulations cannot calculate properly charges in high polar environment, DFT was used to minimize KcsA selectivity filter with different configuration of K^+ and water. All nitrogen atoms were fixed to keep the structure. On both ends were placed 12 water molecules. In case of structures with internal water, one or two of these molecules were swapped for K^+ ion to keep the same number of atoms. Calculated structures included selectivity filter with 3, 4 and 5 K^+ ions (including intracellular and extracellular positions) with and without water between ions.

The most important result: the more K^+ ions are together, the lower is the energy of system The lowest energy have system with occupied places 123W (for structures with 3 K^+), 1234 (4 K^+) and 01234 (5 K^+). The most energetic are 1WE45 (3 K^+) and 0W2W45 (4 K^+). W means water molecule, E – empty/unoccupied position.

Second: boundary ions are more energetic, than ions in the middle of selectivity filter. The intracellular ion (position 5) shows higher energy than extracellular (position 0). Yet the intracellular end was less fixed as Threonine75 OH groups are quite far from fixed N atoms. And the water molecules could converge only in local minima, not the global one – yet the starting structure was the same.

Acknowledgments: The authors gratefully acknowledge the contribution of the Scientific Grant Agency of the Slovak Republic under the grant VEGA 1/0634/25. This work was supported in part through the Comenius University in Bratislava CLARA@UNIBA.SK high performance computing facilities, services and staff expertise of Centre for Information Technology.

[1] Ryan, M. J., Gao, L., Valiyaveetil, F. I., Zanni, M. T., Kananenka, A. A.: Probing Ion Configurations in the KcsA Selectivity Filter with Single-Isotope Labels and 2D IR Spectroscopy, *JACS* **2023** 145 (33), 18529-18537 DOI: 10.1021/jacs.3c05339

Thermal Characterization of Paraffin Candles Modified with Dyes and Fragrances Using DSC

Ewa Muzal[1,2,3], Kinga Wzgarda-Raj[1], Zdzisław Kinart[1]

[1]Department of Physical Chemistry, Faculty of Chemistry, University of Lodz,
Pomorska 163/165, Lodz, Poland
[2]Doctoral School of Exact and Natural Sciences, ul Matejki 21/2, Lodz, Poland
[3]Gala Poland, Fabryczna 10, Wieluń, Poland

e-mail: ewa.muzal@edu.uni.lodz.pl

The aim of this study was to evaluate the impact of colorant and fragrance additives on the thermal properties of paraffin candles using differential scanning calorimetry (DSC). The analysis was conducted on candle samples containing various combinations of functional additives, reflecting the composition of decorative and aromatherapeutic products. Both freshly prepared samples and those subjected to aging under controlled temperature conditions were examined.

DSC measurements enabled the assessment of changes in melting temperature and enthalpy, as well as the crystallization behavior of the tested systems. Comparison with a reference sample revealed that the presence of additives can lead to significant alterations in thermal properties, indicating, among others, unfavorable interactions between components (Figure 1). These findings may serve as a basis for optimizing candle formulations in terms of storage stability and user safety.

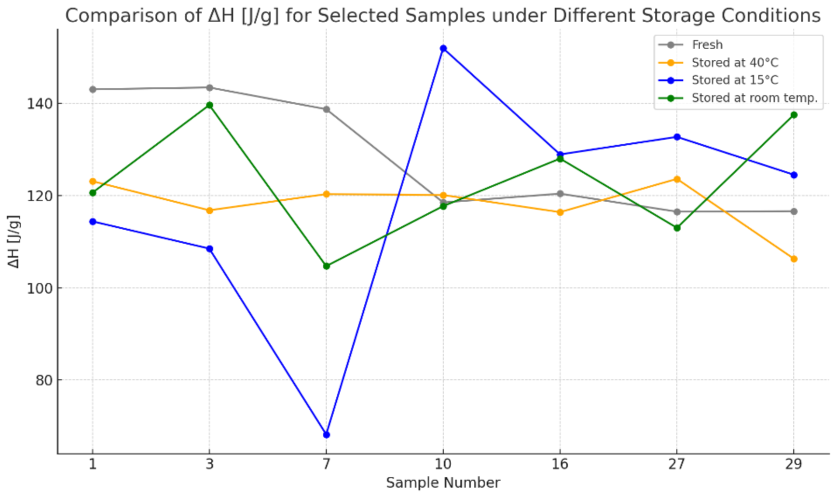


Figure 1. ΔH [J/g] values for selected candle samples stored under different conditions: fresh, 40 °C, 15 °C, and room temperature. Significant variations in the 15 °C group indicate low thermal stability.

Analysis of superstrong hydrogen bonds in thiourea complexes

Aleksandra Rydz, Marcin Palusiak

Department of Physical Chemistry, Faculty of Chemistry, University of Łódź,
Pomorska 163/165, 90-236 Łódź, Poland

The study presents structural an energetic analysis of selected interactions observed in the crystal structures of thiourea unoxidized and oxidized analog. A comparison of the structural parameters of both thiourea forms was performed. The analysis of topological parameters such as electron density at the bond critical point (ρ) and its Laplacian ($\nabla^2\rho$) indicates a shift in the character of the C–S bond towards a more ionic nature in the oxidized form.

Additionally, many-body interaction effects were analyzed using the M06-2X/aug-cc-pVTZ, including the counterpoise correction for basis set superposition error. This method allowed for estimating the contribution of non-additive many-body effects, with BSSE-corrected values ranging from 0.5 to 2 kcal/mol. The non-additive contribution, calculated as the difference between the total complexation energy and the sum of pairwise interactions, confirms a moderate impact of many-body effects on the stability of the studied complexes.

In the analyzed crystal structures, hydrogen bonds are clearly observed to act as stabilizing bridges. Both the geometry of the systems and the complexation energies, ranging from –21.7 kcal/mol to –98.9 kcal/mol, confirm the exceptional strength of these interactions and their influence on the spatial arrangement and overall stability of the structures. Analysis of non-additive contributions shows that the tetramer is affected most significantly by many-body effects (–7.23 kcal/mol), confirming the presence of synergistic interactions. Topological and energetic characterization indicates that the oxidized thiourea system promotes the formation of superstrong hydrogen bonds.

	Dimer	Trimer	Tetramer
Corrected complexation energy [kcal/mole]	-21,69	-41,99	-98,97
Non-additive contribution	-	-1,16	-7,23

Table 1: The values of complexation energies in dimer, trimer and tetramer thiourea crystal complexes after BSSE correction and non-additive contributions in trimer and tetramer.

[1] M. Domagała, S. Simon, M. Palusiak, Int. J. Mol. Sci. 23 (2022) 233.
[2] G. Gilli, P. Gilli, J. Mol. Struct. 552 (2000) 1–15

The impact of visible light and darkroom conditions on the crystallization of systems containing trithiocyanuric acid

Marcin Wlaźlak, Kinga Wzgarda-Raj

University of Łódź, Faculty of Chemistry, Pomorska 163/165, 90-149 Łódź, Poland

Trithiocyanuric acid is an aromatic compound with three-fold symmetry,[1] containing three proton-donor groups (N–H) and three proton-acceptor groups (C=S).[2] The presence of these functional groups gives the molecule a strong capacity for binding heavy metal ions.[3]

This study aimed to investigate the influence of electromagnetic radiation on the crystallization process of chemical compounds and the resulting crystal structures. As a result of the experiments, four new co-crystals were obtained, which are not deposited in the Cambridge Structural Database (CSD).[4] (Fig. 1). Furthermore, it was found that light exposure conditions significantly affect the crystallization process, leading to the formation of different crystal structures from the same compounds.

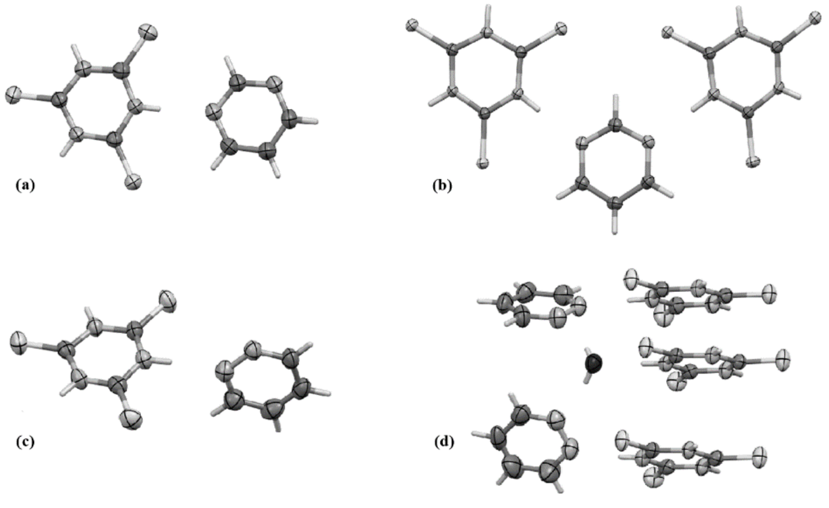


Figure 2: The diagram illustrates the molecular arrangement in the co-crystal structures of trithiocyanuric acid with pyrimidine (a, b) and pyridazine (c, d), obtained under visible light irradiation (a, c) and darkroom conditions (b, d), respectively.

[1] P. A. W. Dean, M. Jennings, T. M. Houle, D. C. Craig, I. G. Dance, J. M. Hook, M. L. Scudder, CrystEngComm, 6 (2004) 543-548.
[2] N. Osaka, M. Ishitsuka, T. Hiaki, Journal of Molecular Structure, 921 (2009) 144-149.
[3] M. Heidari, K. Ghanemi, Y. Nikpour, Ecotoxicology and Environmental Safety, 204 (2020) 110995
[4] C.R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, Acta Crystallographica, Section B, 72 (2016) 171-179.

Hydrogen bonding patterns in trithiocyanuric acid cocrystals: structural, topological, and energetic analysis into N–H···S interactions

Kinga Wzgarda-Raj

Department of Physical Chemistry, Faculty of Chemistry, University of Lodz,
Pomorska 163/165, 90-236 Lodz, Poland

This study presents the crystal structures of four newly obtained cocrystals of trithiocyanuric acid (TTCA) with diazine derivatives, emphasizing the role of N–H···S hydrogen bonds in stabilizing supramolecular architectures. TTCA forms two distinct chain motifs—linear and zigzag—both built around the $R^2_2(8)$ hydrogen-bonding synthon. Single-crystal *X*-ray diffraction combined with Hirshfeld surface analysis confirms that these arrangements are structurally viable and reflect the inherent supramolecular preferences of TTCA.

To better understand the energetics of these assemblies, a quantum chemical approach was employed, including topological analysis and many-body energy decomposition of intermolecular interactions. The findings underscore the key role of hydrogen bonds involving amine groups in stabilizing the structures and shed new light on the relationship between molecular architecture and interaction energy in cocrystal systems.

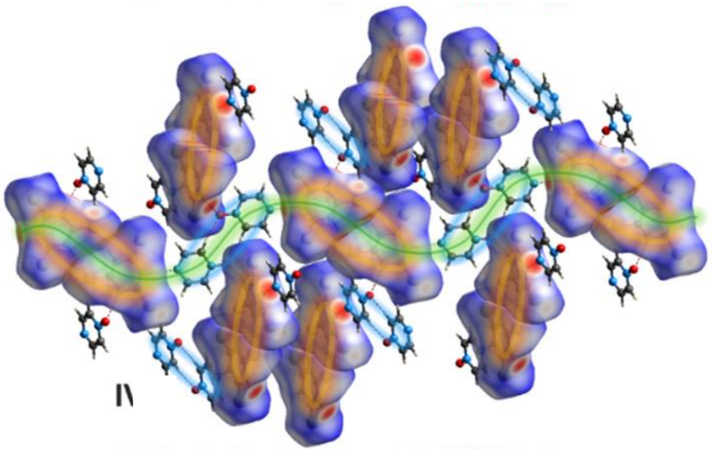


Figure 1. Hirshfeld molecular surfaces in cocrystal showing supramolecular motifs stabilized by homo- and heteromolecular N–H···S hydrogen bonds.

[1] Wzgarda-Raj, K.; Rybarczyk-Pirek, A.; Palusiak, M. *CrystEngComm*. **2025**, 27, 784–794.