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Program

Thursday, January 22

8:30–9:00	**Registration**	
9:00–9:10	**Mindaugas Mačernis**	Welcome words
9:10–9:30	**Juozas Šulskus**	Modelling urea-biuret-water solutions for NIR spectroscopy
9:30–9:50	**Žyginta Murnikova**	Modeling Peptides in Aqueous Ionic Liquid Mixtures: a Quantum Mechanics/Molecular Dynamics Study of Structural and NMR Properties
9:50–10:10	**Kęstutis Aidas**	Towards accurate modelling of 1H NMR spectra of ionic liquids: The case of [C4mim][BF4] and its aqueous mixtures
10:10–10:30	**Rokas Garbačauskas**	HIDRA – a Hierarchical DFT accuracy transformer model to Reconstruct Atomic geometry
10:30–10:50	**Coffee break**	
10:50–11:20	**Bruno Robert** **(Invited speaker)**	Carotenoids: from ground-state modelling to access to excited manifold
11:20–11:40	**Lena Golubewa**	Hyperspectral fluorescence imaging of desiccation tolerant desert moss *Syntrichia caninervis*: tracking the rapid recovery of photosynthetic machinery during rehydration
11:40–12:00	**Gabrielė Rankelytė**	Protein-Controlled Electronic Energy Transfer in PSI
12:00–13:00	**Lunch**	
13:00–13:30	**Darius Abramavičius**	Off-resonant nonlinear optical spectroscopy and its application to two-dimensional electronic spectroscopy
13:30–13:50	**Arunjyoti Baidya**	A tunable framework for vibronic dynamics: Generalized nonlinear exciton equations
13:50–14:10	**Valdas Jonauskas**	Theoretical study of electron-impact ionization for W^+ ion
14:10–14:30	**Einaras Sipavičius**	Molecular dynamics / quantum mechanics modelling of aqueous mixtures of choline tryptophanate ionic liquid
14:30–14:50	**Alytis Gruodis**	Protonation of the $TPPS_4$ center due to Interactions with *L*-Ascorbic acid. Simulations using the DFT approach
14:50–15:20	**Photo** **Coffee break**	
15:20–15:40	**Jelena Tamulienė**	How to improve the optical properties of a pyridinium luminophore: Theoretical study
15:40–16:00	**Ivan Halimski**	Optical properties of *trans*-stilbene under various conditions
16:00–16:20	**Rokas Dobužinskas**	Hidden Amorphous Phase Evolution in Stilbene–Polystyrene Composites Revealed by X-ray Diffraction
16:20–16:45	**Mindaugas Mačernis**	Molecular Dynamics-Based Structural Sampling: Case Studies of Stilbene, Urea, and Carotenoid Complexes
17:00–19:00	**Networking (Dinner)**	

Welcome

We are pleased to welcome you to the 6th EuroCC Vilnius workshop on HPC usage, organized by the Lithuanian National Competence Centre (NCC Lithuania) under the EuroCC4SEE project. This event will cover various research topics utilizing High-Performance Computing (HPC) resources, including the Vilnius University supercomputer ‘VU HPC’ Saulėtekis at the Faculty of Physics and EuroHPC facilities. Topics will range from experimental data treatment to quantum chemistry and molecular dynamics, alongside discussions on potential academia-industry collaborations. We wish you inspiring presentations, fruitful discussions, and enjoyable networking opportunities.

The Organizers

Modelling urea-biuret-water solutions for NIR spectroscopy

Juozas Šulskus[1], Vytautas Bubilaitis[1], Raimundas Steponavičius[2], Mindaugas Mačernis[1]

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The study investigated complexes formed by urea, biuret, and water molecules in an aqueous solution, as well as the relative stability of these complexes and their excited vibration spectra in the IR spectrum range (12500–4000 cm-1 or 800–2500 nm). Such studies are important for the use of NIR spectrometry in real-time analysis of concentrated "non-ideal" solutions.

It is known that changes in urea concentration and solution temperature result in the formation of urea molecule complexes of varying sizes, as well as urea-biuret complexes, with these compounds simultaneously forming hydrogen bonds with water molecules (Fig. 1). As the temperature increases, the urea molecule complexes decrease in size and practically only urea-urea dimers remain. One of the main objectives is to evaluate what intermolecular complexes are formed at different solution concentrations and temperatures and to determine the relative number of these molecular complexes in the solution. This task was solved by solving the molecular dynamics problem.

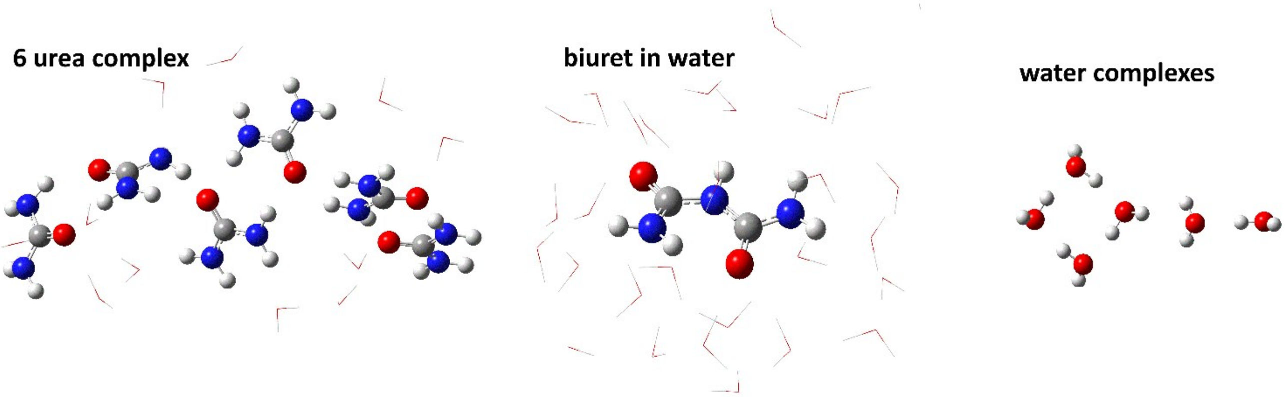

Fig. 1. Molecular complexes in urea and biuret in water solution.

To evaluate the stability of the resulting molecular complexes, their geometric parameters, and excited vibration spectra, computer calculations were performed using Gaussian 16 [1] and Gamess US [2] software.

The calculations were performed using the resources of the Saulėtekis supercomputer at Vilnius University's Faculty of Physics. This work is part of the Lithuanian Science Council's Eureka network Applied Quantum Technologies Project No. 10-052-P-01-012.

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Modeling Peptides in Aqueous Ionic Liquid Mixtures: a Quantum Mechanics/Molecular Dynamics Study of Structural and NMR Properties

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Ionic liquids (ILs) have been known as "green" and biocompatible solvents for quite some time and some of their possible biological uses include changing catalytic activity of enzymes, stabilizing or destabilizing various proteins, as well as making them permeate more easily through membranes [1]. The nature of ILs and proteins interactions varies and is difficult to evaluate, so smaller peptides are often used as a model system to discover how different ILs interact with said peptides and change their structure in the aqueous solution. The method most suited for recognizing intermolecular interactions is nuclear magnetic resonance (NMR) spectroscopy as atoms, especially hydrogen, chemical shift is very sensitive to changes of central molecule's close environment.

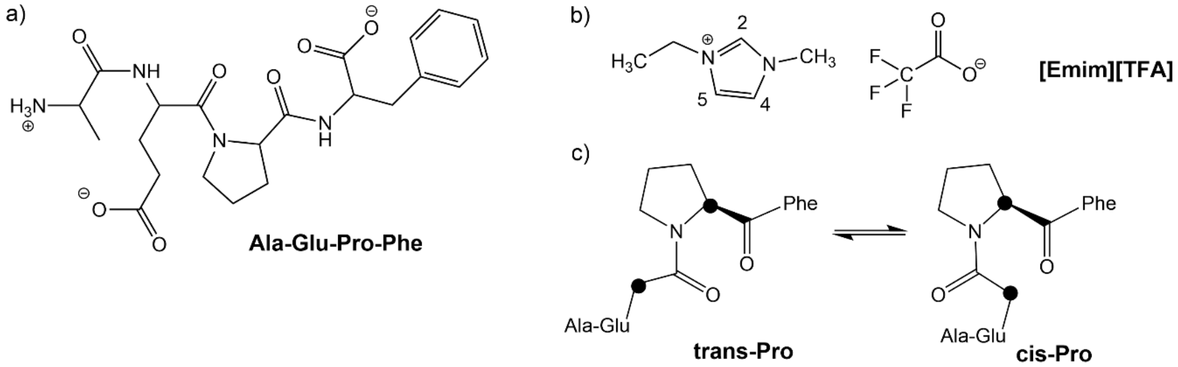

Fig. 1. Structural formulas of a) peptide Ala-Glu-Pro-Phe, b) ethyl-3-methylimidazolium trifluoroacetate, c) *trans/cis* isomeric forms of AEPF

In this work an Ala-Glu-Pro-Phe tetrapeptide (AEPF) was investigated using molecular dynamics (MD) simulations and quantum mechanics/molecular mechanics calculations, while in an aqueous environment and in IL/water mixture. An ionic liquid consisting of a popular imidazolium cation and trifluoroacetic acid – ethyl-3-methylimidazolium trifluoroacetate ([Emim][TFA]) was chosen. This peptide exists in two different isomers due to proline amino acid – *cis* or *trans,* both of them were evaluated. Theoretically computed chemical shift differences of peptide's hydrogen atoms were compared to experimental results [2] allowing us to evaluate the different interactions taking place in peptide/IL/water systems, while MD simulation data revealed some structural changes in the peptide's structure itself.

ACKNOWLEDGEMENTS

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Towards accurate modelling of ^{1}H NMR spectra of ionic liquids: The case of [C4mim][BF4] and its aqueous mixtures

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Room-temperature ionic liquids (ILs) are organic salts that remain liquid near ambient conditions and are widely studied for their unique physicochemical properties. However, their locally anisotropic structure and nanoscale segregation complicate structural analysis using ^{1}H NMR spectroscopy. Earlier attempts to model proton chemical shifts of imidazolium-based ILs using single ion-pair models reproduced only qualitative spectral features.

In this work, an integrated approach combining molecular dynamics (MD) simulations and QM/MM calculations is applied to accurately predict ^{1}H NMR spectra of 1-butyl-3-methylimidazolium tetrafluoroborate (C4mim][BF_4]) and its aqueous mixtures (IL molar fraction 0.17–1). Classical MD simulations with an IL-specific force field were used to characterize local structure, followed by QM/MM calculations of isotropic ^{1}H shielding constants.

MD results show that BF_4^- anions preferentially localize near the C2–H2 site of the imidazolium ring rather than above the ring, contradicting earlier experimental assumptions. Even at low IL concentrations, water molecules rarely displace anions from the first solvation shell around C2–H2, leading to a relatively stable local environment. Nanosegregation is observed: butyl chains form nonpolar domains, while water accumulates in anion-rich regions.

The calculated ^{1}H chemical shifts agree closely with experiment, with deviations of only ~0.2 ppm across all systems. The notoriously difficult-to-predict H2 proton shift is reproduced with high accuracy. Overall, the ^{1}H NMR spectra of the [C4mim]$^+$ cation remain nearly composition-independent despite structural changes in the mixtures.

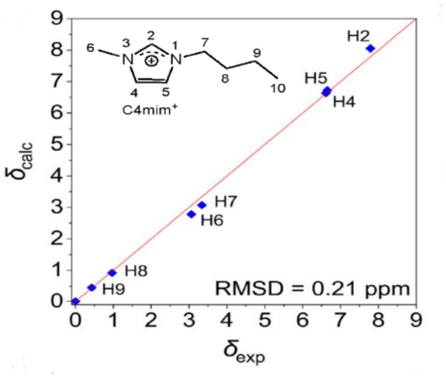

Fig. 1. Comparison between the calculated and measured relative ^{1}H NMR spectra of C4mim$^+$ cations in pure C4mim][BF_4]. The experimental and calculated ^{1}H NMR chemical shift values, denoted as δ_{exp} and δ_{calc}, are given in ppm [2].

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HIDRA – a Hierarchical DFT accuracy transformer model to Reconstruct Atomic geometry

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Predicting molecular properties from string representations enables high-throughput screening without expensive 3D structure generation. We present a systematic comparison of SMILES [1] and SELFIES [2] representations using transformer encoders [3] trained on 3.9 million DFT-optimized molecules from the PubChemQC database, predicting seven structural and symmetry properties.

This work addresses three questions: which string representation better encodes molecular structure for property prediction, how transformer depth should scale given limited quantum chemistry data, and whether multi-task learning improves performance through shared representations. We evaluate three architectural variants shown in Fig. 1: single-task models with one property per encoder, parallel multi-task with all prediction heads at the final layer, and hierarchical multi-task with heads at different encoder depths and cross-attention feedback between properties.

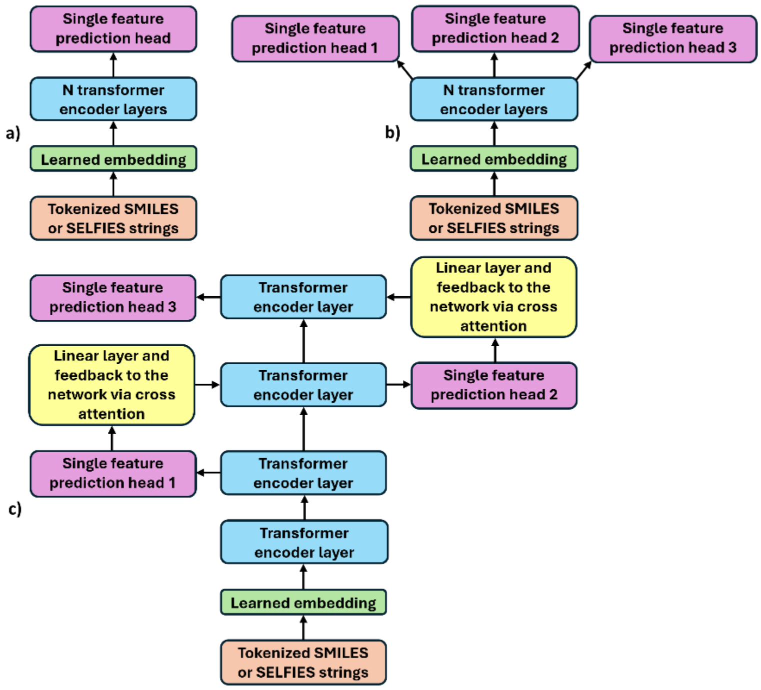

Fig. 1. (a) Single-property, (b) parallel multi-property, and (c) hierarchical multi-property transformer encoder networks.

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Carotenoids: from ground-state modelling to access to excited manifold

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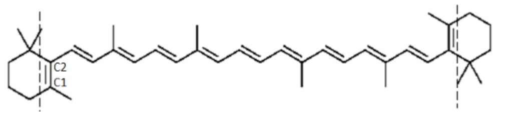
Carotenoid molecules are linear, highly conjugated molecules, with many roles in biology ranging from light-harvesting and photoprotection in photosynthesis, to signaling in fruits and flowers, precursors of plant growth hormones and vitamin A (retinal) or retinol, an essential driver of fetal development.



Structure of β-carotene

Despite their apparent simplicity, carotenoid molecules turn out to be difficult to model with precision, and they actually can be used to benchmark modelling approaches as their electronic and vibrational properties can be easily characterized in detail[1,2]. We are now able to predict with accuracy the properties of quite complex molecules from the carotenoid family[3,4].

Our next goal now resides in modelling carotenoid excited states. Here again, it turns out that the photochemistry of these molecules is much more complex than initially predicted. Only last year were we able to determine with precision the cascade of energy transfers following the photon absorption by these molecules, and we could as well characterize the vibronic properties of each electronic state involved[5]. We aim now to use this information to build-up a comprehensive model of carotenoid electronic properties and photochemistry.

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Hyperspectral fluorescence imaging of desiccation tolerant desert moss *Syntrichia caninervis*: tracking the rapid recovery of photosynthetic machinery during rehydration

Lena Golubewa[1,2], Yaraslau Padrez[1,3], Andrius Gelžinis[1,2], Kipras Mažeika[4], Augustas Vaitkevičius[4,5], Simona Streckaitė[1], Jevgenij Chmeliov[1,2], Vilius Čirgelis[1], Chunhong Yang[6], Leonas Valkūnas[1], Bruno Robert[7]

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Syntrichia caninervis (*S. caninervis*) is one of the dominant species in moss crusts. It is characterized by remarkable tolerance to extreme environmental conditions [1]. The mechanisms of the rapid (from seconds to minutes) recovery of its photosynthetic function gain a lot of interest. Hyperspectral imaging of the moss leaves in dehydrated and rehydrated state may shed light on the specificity of the pigment redistribution in the leaf cells upon recovery. In the present study, hyperspectral imaging of *S. caninervis* was performed at the micro- and macroscopic scales. To reveal the spatial heterogeneity in spectral characteristics over the leaf area in dehydrated and rehydrated leaf cells of *S. caninervis* and identify the patterns of spectral features within the leaf, image segmentation based on the corresponding spectral datasets was performed. Hyperspectral image segmentation was done by *k*-means clustering. The number of clusters was determined based on the combination of three segmentation quality metrics. Significant spectral heterogeneity was revealed in both dehydrated and rehydrated moss samples at the micro- and macroscopic levels. Both dehydrated and rehydrated moss samples show fluorescence in the 530-650 nm range, with dehydrated samples exhibiting significantly higher relative intensity and variance in the fluorescence peak position than rehydrated moss leaves, probably resulting from partially disassembled pigments, e.g. carotenoids. The intensity ratio I_{685}/I_{740} varies in both the dehydrated and rehydrated samples, but is much lower in the dehydrated sample, indicating the dominance of photosystem (PS) I. However, the fluorescence emission peaks related to PSII (685 nm) are also present and more pronounced in the edge clusters, probably indicating the contact of these areas with humid air and the onset of PSII recovery. The gradual shift of the peak from 690 nm to 707 nm when moving the outer segments towards the inner parts of the dehydrated moss leaf could refer to different phases of PSII recovery.

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Protein-Controlled Electronic Energy Transfer in PSI

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Photosystem I (PSI) is the most efficient light-to-energy conversion apparatus. To reach and maintain high quantum yield, all processes in PSI, including electronic energy transfer (EET) between the pigments, must be exceptionally rapid. After the absorption, excitation energy can be transferred to the nearby pigment over tens of angstroms. Such dynamics is determined by inter-pigment couplings J_{mn}, described in terms of the electronic transition densities [1], that can be replaced by the atomic transition charges [2]. We have investigated the excitation dynamics in four complexes of PSI light-harvesting antenna LHCI (see Fig. 1). The structure of the antenna was obtained from the PDB (PDB ID: 5L8R) [3]. We used the aforementioned approach to obtain the chlorophyll-chlorophyll coupling energies in vacuum and in protein environment. For accounting for the protein environment, we used similar approach to our previous research [4]. We have also accounted for the solvent screening effect [5] and compared the properties of EET with the effects of protein and solvent screening and without (vacuum).

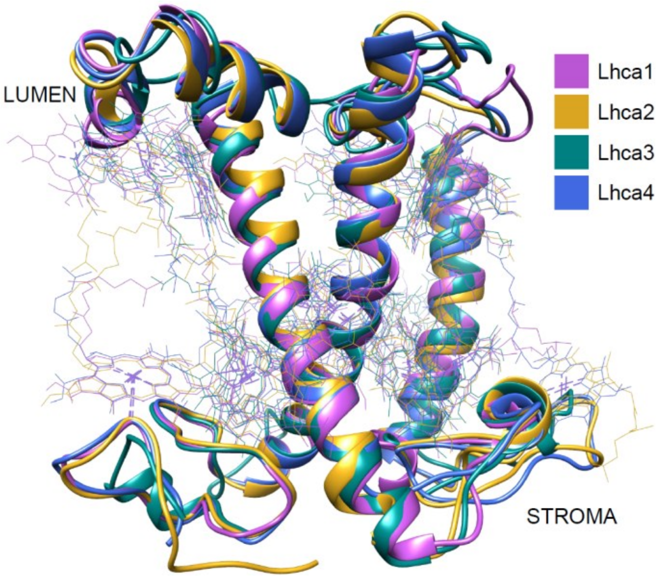

Fig. 1. Lhca1-4 complex structures mapped on top of each other.

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Off-resonant nonlinear optical spectroscopy and its application to two-dimensional electronic spectroscopy

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At the resonant conditions various kinds of spectroscopy can be easily associated with different types of Feinman diagrams, which describe the sequence of interactions, which lead to the specific type of nonlinear optical measurement. However, the situation is much more complicated in off-resonant conditions. In that case all types of interaction sequencies may have comparable amplitude and all of them should be summed up in signal calculations. That is the case for example in second harmonic generation (SHG) measurement in transparent medium. In principle it is then not clear whether signal is generated from vibrational or electronic degrees of freedom and that is still the open question in e.g. SHG of proteins. Often partially off-resonant conditions may be realized, what is the case for third order nonlinear spectra measurement in e.g. two-dimensional electronic spectroscopy (2DES). In this presentation we present the off-resonant calculation scheme for 2DES spectra of transparent medium. We demonstrate that vibrations of the solvent can have a measurable effect in the measurement of solutions and can contribute to the “real” signal as a systematic non-random “noise” leading to nicely structured 2DES spectra as demonstrated in Fig. 1.

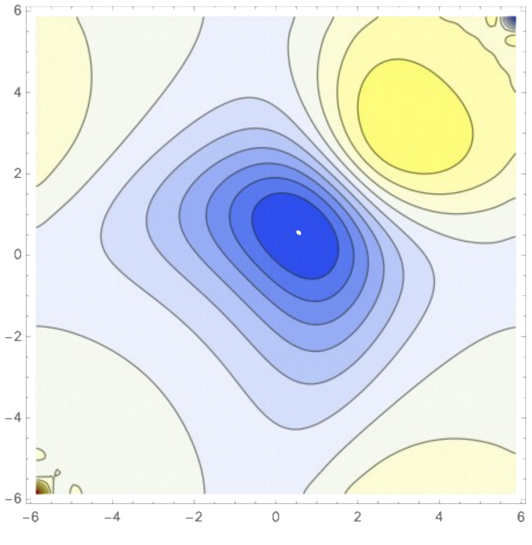

Fig. 1. 2DES spectrum of liquid water calculated in off-resonant “transparent” window.

A Tuneable Framework for Vibronic Dynamics: Generalized Nonlinear Exciton Equations

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Accurately modeling coupled electronic–vibrational dynamics in molecular aggregates is essential for interpreting energy transfer and nonlinear optical signals. We present a non-perturbative framework based on Generalized Nonlinear Exciton Equations (NEE) derived from the Heisenberg equation for a Frenkel-exciton Hamiltonian. A central feature is a generalized commutation scheme introducing a single parameter η that continuously interpolates between bosonic and paulionic statistics, enabling flexible descriptions beyond either limit. The formalism rigorously treats a linearly coupled harmonic bath, yielding a closed hierarchy for exciton populations or coherences and mixed exciton–phonon correlations.

We position two practical closures within this hierarchy. First, the Mean-Field Approximation (MFA)—a full factorization of exciton–phonon averages—recovers a limit in which quantum excitons evolve in an effectively classical bath; we quantify regimes where MFA is accurate and where it breaks down. Second, the 1-Quantum Approximation (1QA) retains only single-quantum vibrational excitations and the leading exciton–phonon coherences; we use 1QA as a controlled reduction that preserves vibronic resonances at moderate cost.

As an application, we provide preliminaries for the bacterial reaction center (BRC): site-based Hamiltonian construction for the special pair and accessory pigments and the transition-dipole orientations taken from structure.

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Theoretical study of electron-impact ionization for W^+ ion

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Tungsten is commonly used as a plasma-facing material in tokamak fusion devices because it has a very high melting point and resists erosion. However, collisions with high-energy plasma particles can release tungsten atoms and ions into the plasma. These heavy impurities increase radiation losses and reduce plasma performance. Therefore, accurate ionization cross sections are important for plasma modeling, diagnostics, and predicting impurity behavior under different operating conditions.

Aim of the current work is to analyze single ionization cross sections for the W^+ ion using the scaled distorted wave (sDW) approximation [1]. The analysis includes energy levels of the ground $5d^46s$ configuration of the W^+ ion. The sDW results are compared with experimental data [2, 3] and distorted wave (DW) calculations.

Radial orbitals for considered configurations of tungsten ions are calculated using the Flexible atomic code (FAC) [4] where coupled Dirac equations are solved for a local central potential. Transitions are analyzed among configurations of the W^+ and W^{2+} ions. Excitation cross sections to the autoionizing configurations are estimated in order to determine excitation-autoionization (EA) contribution. In addition, the radiative and Auger rates from these subconfigurations are calculated to evaluate autoionization branching ratios for the produced subconfigurations. The DW approximation is used to calculate the direct ionization (DI) and excitation cross sections [4].

DI process includes the 5d and 6s subshells for the $5d^46s$ configuration. DI from the deeper subshells of the studied configuration produces autoionizing configurations that are above the double ionization threshold. These excited autoionizing configurations primarily decay through autoionization and, therefore, result in higher ionization stages than W^{2+}.

The first step of the EA process is analyzed for excitations from the 4f, 5d, and 6s subshells of the $5d^46s$ configuration. The excitations up to shells with the principal quantum numbers $n \leq 30$ and orbital quantum number $l \leq 5$ are included in the study.

The DI process dominates for all studied energy levels and contributes $\sim 80\%$ to the total ionization cross sections. EA channels corresponding to excitations from the 5d subshell dominate over the EA 4f and EA 6s channels for all energy levels of the ground configuration.

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Molecular dynamics / quantum mechanics modelling of aqueous mixtures of choline tryptophanate ionic liquid

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Choline tryptophanate [Cho][Trp] is a biocompatible, biodegradable ionic liquid belonging to choline-aminoacid family of ionic liquids ([Cho][AA] ILs). The potential for applying [Cho][AA] ILs in biomass processing and pharmaceutical fields stems from their ability to effectively solubilize some macromolecules (e.g. lignin [1]) and drugs (e.g. glibenclamide [2]) in aqueous medium. Nanoheterogeneity of [Cho][AA] IL-water mixtures is believed to be an important feature in solubilization process. Choline lysinate [Cho][Lys] was expected to not have nanodomain-like structure, shown by X-ray diffraction measurements [3], but neutron scattering and our theoretical study supported the formation of polar and nonpolar domains [1,4]. Therefore we aim to scrutinize the intermolecular structure of aqueous mixtures of another [Cho][AA] IL – choline tryptophanate, which should also be non-nanosegregated, according to X-ray diffraction experiments [3].

In order to get information about local coordination around each moiety of Cho^+, Trp^- and H_2O, and aggregate size distribution, we performed molecular dynamics (MD) simulations of two [Cho][Trp]:H_2O mixtures (one having 10 % [Cho][Trp] molar fraction and another having a single ionic pair surrounded by 4000 water molecules). ^1H NMR shielding constants of some nuclei in Cho^+ and Trp^- were calculated with qualitative precision by conducting quantum mechanics / molecular mechanics (QM/MM) calculations on 100 configurations extracted from MD trajectories.

We would like to thank to "HPC Sauletekis" for providing us computational resources.

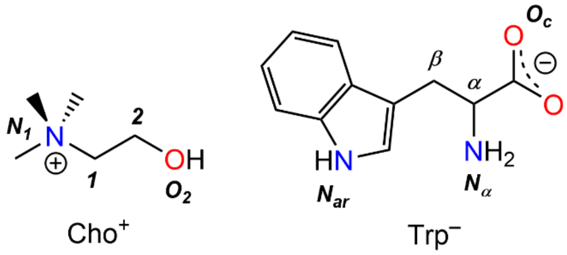

Fig. 1. Choline tryptophanate [Cho][Trp] chemical structure and important atomic labels.

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Protonation of the $TPPS_4$ center due to Interactions with *L*-Ascorbic acid. Simulations using the DFT approach

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In the class of naturally occurring porphyrins, tetrakis (4-sulfonatophenyl) porphyrin ($TPPS_4$, H_2TPP, see Fig. 1, top, M1**)** represents heterocyclic compound which is important as a potential photosensitizer for production of the singlet oxygen [1] (cancer photodynamic therapy). Modeling results presented in Ref. [2] showed that geometry of $TPPS_4$ molecule changes from flat (ionic form at neutral pH), to saddle-shaped (protonated core at moderate acidity) ionic forms ($H_2TPPS_4^{4-}$, $H_4TPPS_4^{2-}$, $H_6TPPS_4^{0}$, and $H_8TPPS_4^{2+}$). *L*-Ascorbic acid (vitamin C, hexuronic acid, see Fig. 1, bottom, M3) represents well-known organic material of high biological importance. *L*-Ascorbic acid could be used as antioxidant for help protect against oxidative stress in tissues and inflammation [3]. This work is dedicated to the study of modeling the interaction of $TPPS_4$ (M1) and L-ascorbic acid (M3).

Simulations. Several complexes such as M4 and M5 were used for simulations.

M4= M3+M1; M5= M3+M1+M3.

Gaussian16 [4] package was used to establish the ground state complex structure and corresponding electronic excitations. Optimization in the ground electronic state has been provided using semiempirical CAM-B3LYP method and 6-31G(d) basis set consisting of polarization function (d). Electronic excitations were calculated using semiempirical TD method for singlets only. Environmental effects were included using PCM (water) routine for structure simulations as well as for excitations. Fig. 2a and b represents M4 complex and M5 complex respectively. Both structures are presented in two projections after optimization using CAM-B3LYP/6-31G(d) method. Solvation effects using PCM(water) were included. Firstly, for M4 and M5 complexes, M1 monomer was presented in centre-unprotonated flat form (two protons at centre only) which corresponds to case of neutral surrounding at pH=7. M3 monomer was presented as *L*-ascorbic acid (two protons in positions 4 and 5). Successful optimization in the ground electronic state allows obtaining the weak associate without geometry change (M1 flat, centre protonated by two native protons) and without proton transport (M3 in form of *L*-ascorbic acid, reduced form). Secondly, additional structure optimization in the first excited electronic state allows obtaining weak associate with geometry change (M1 saddle-shaped, centre fully protonated, four protons) and proton transport is present (M3 in form of *L*-dehydroascorbic acid, oxidized form). This final situation is depicted in Fig. 2. In case of M4 complex (one *L*-ascorbic acid), protons of *L*-Ascorbic acid from position 4 and 5 (two per one molecule) must be shared between *L*-Ascorbic acid and $TPPS_4$. In case of M5 complex (two *L*-ascorbic acids), two necessary protons (one per each molecule) were present in proton transfer.

Conclusions. Simulation of the molecular structures using quantum chemical methods allows to estimate most probable structures of separate monomers *L*-Ascorbic acid and $TPPS_4$ as well as the complexes. Initial hypothesis about the role of *L*-Ascorbic acid as reducing agent when neighbour contact to $TPPS_4$ is present was approved. In complex [*L*-Ascorbic acid + $TPPS_4$ + *L*-Ascorbic acid], intermolecular charge transfer takes place. Protonation of centre of $TPPS_4$ could be provided using two *L*-Ascorbic acids as the proton sources. Presence of *L*-Ascorbic acid in the solvent allows protonation reaction in form of $TPPS_4 \rightarrow H_2TPPS_4$.

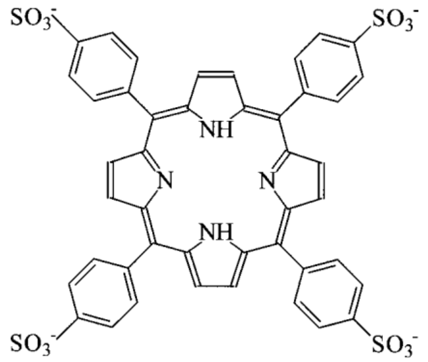	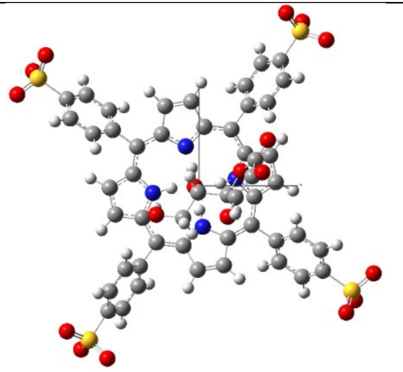	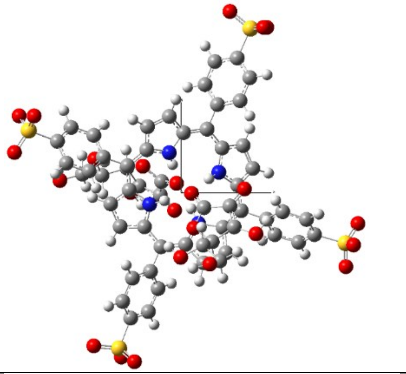
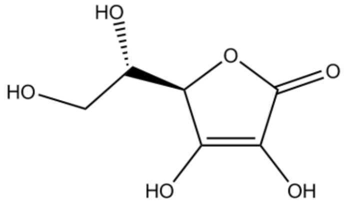	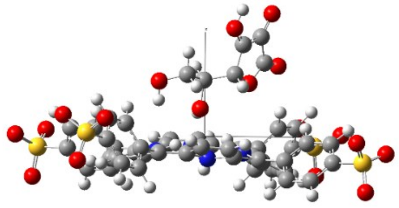	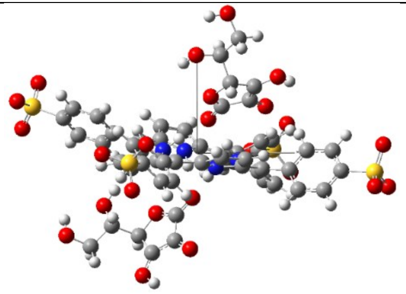
Fig. 1. Structures of monomers. Top – **M1**, Tetrakis (4-sulfonato-phenyl) porphyrin (TPPS$_4$, H$_2$TPP). Bottom – **M3**, *L*-Ascorbic acid (vitamin C, hexuronic acid).	Fig. 2a. Complex **M4=**M3+M1. XY (top) and XZ (bottom) projections. Structures after optimization using CAM-B3LYP /6-31G(d) method. Solvation effects using PCM(water) were included.	Fig. 2b. Complex **M5=**M3+M1+ M3. XY (top) and XZ (bottom) projections. Structures after optimization using CAM-B3LYP/6-31G(d) method. Solvation effects using PCM(water) were included.

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How to improve the optical properties of a pyridinium luminophore: Theoretical study

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In recent decades, sensors have become valuable tools in our lives. The application of sensors is broad, ranging from measuring temperature to alarming the presence of harmful materials in the environment. These different applications lead to a variety of sensors occurring due to their advantages in certain situations. For example, in a harsh environment, non-contact high-precision measurements are performed mostly by optical sensors, where the luminophore is a critical component, as it directly affects the sensor's ability to detect target analytes or environmental changes.

Recently, we obtained that the KL 1421 luminophore exhibits selective sensing behavior toward acetic acid vapors, as no significant photoluminescence response was observed for other tested substances. Hence, we concluded that the incorporation of carotenoids could lead to an increase in the molar absorptivity of the luminophore, which leads to an increase in its absorption efficiency and improving the sensitivity of the optical sensor, provided that photoluminescence quantum yield and other photophysical properties remain favorable.

The geometry, its change, and the charge redistribution in KL 1421 when the molecule interacts with carotenoids and/or sensed molecules such as NH_3 and acetic acid were studied by the B3LYP/cc-pVTZ approach. The orbital diagrams were used to illustrate the excitations and their variations resulting from the formation of the above complexes. The increase in molar absorptivity is observed in compounds with carotenoids, leading to higher absorbance of KL 1421. The results of our investigations exhibit that conjugated double-bond number influences charge redistribution in the KL 1421 & carotenoid & sensed molecule compounds. The strong interactions of KL 1421 and carotenoids, and KL 1421 & carotenoids with sensed molecules were observed. The results of our investigation prove that NH_3 could not be sensed by KL 1421, although it could be possible by KL 1421 & carotenoid due to the energy level variations and the shifts of the peaks corresponding to the excitations due to charge transfer from the sensed molecule. We also found that in the KL 1421 & carotenoids & sensed molecule, the triplet state is closer to the singlet one. Hence, the singlet-triplet transfer in the compounds with carotenoids will be faster than that in the KL 1421 & sensed molecule, while the transfer from the triple state to the ground one is longer and more efficient. The molar absorptivity indicates higher absorbance of the compound under study with carotenoids than without them. Additionally, the analysis of oscillator strength reveals that the strong interaction among species in KL 1421 & carotenoids could facilitate radiation emission.

In conclusion, the carotenoids are a good choice to improve the sensory properties of KL 1421 - novel organic luminophores.

Optical properties of *trans*-stilbene under various conditions

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Trans-stilbene (TS) is an organic compound ($C_{14}H_{12}$) demonstrating *trans-cis* photoisomerization in a liquid form and morphology-dependent optical properties when it is solid [1, 2]. TS crystals are utilized for the detection of ionizing and ultraviolet radiation. Additionally, TS, being non-polar, serves as a good model system to reveal features of van der Waals (vdW) interaction between organic compounds and 2D materials, such as hexagonal boron nitride (hBN) [3]. TS derivative, *trans*-resveratrol (RSV), exhibits anticancer and antifungal activities, therefore RSV/hBN vdW complex can be considered as a model drug delivery system due to potential hBN applications as a delivery platform. Such applications as photovoltaics, artificial photosynthesis and optoelectronics also require understanding of both morphology-dependent phenomena and the manifestation of vdW interaction between organic compounds and inorganic 2D materials, as well as their interplay.

The study explores optical properties of different phases of solid TS: monomolecular, aggregated and monocrystalline spin-coated films. We study these films by varying both thickness (from 45 nm to 670 nm) and TS concentration (from 0.5% to 80%) with UV/vis absorption and fluorescence, while the films morphology are explored with atomic force microscopy and coherent anti-Stokes Raman scattering. Another focus of the study is vdW interaction between non-polar TS and hBN, as well as between polar RSV and hBN. We study these complexes with THz, IR, UV/vis spectroscopies and with Raman scattering.

Deep insights into TS under different conditions are provided. With the increase in its concentration in polystyrene films a smooth transition from monomolecular properties to those of monocrystals is observed, therefore sample preparation procedure provides fine control of both morphology and optical properties of the film. Manifestation of vdW interaction between TS (RSV) and hBN, most effectively observed with Raman scattering, results in subtle changes in optical properties of the former due to the modification of their electronic clouds. Additional insights are provided with density functional theory calculations.

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Hidden Amorphous Phase Evolution in Stilbene–Polystyrene Composites Revealed by X-ray Diffraction

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X-ray diffraction studies of molecularly doped polymers are commonly focused on the appearance and growth of crystalline peaks, while changes in the amorphous polymer matrix are often treated as a static background. In this work, we show that the amorphous phase itself undergoes a systematic transformation in stilbene–polystyrene composites, which becomes evident only when analyzed beneath the dominant crystalline reflections.

Polystyrene films containing different concentrations of stilbene were investigated by X-ray diffraction under identical preparation conditions. As expected, increasing stilbene concentration leads to the emergence and strengthening of diffraction peaks associated with crystalline stilbene domains [1,2], from which characteristic crystallite sizes were estimated. However, in parallel, a broad amorphous halo attributed to polystyrene remains present in all spectra and changes markedly with dopant concentration.

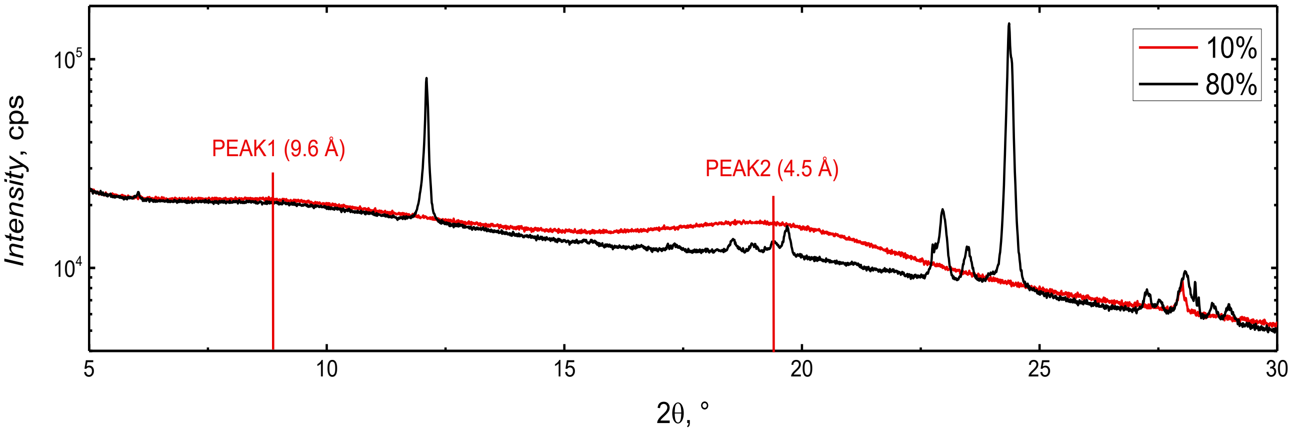

Fig. 1. XRD spectra of 10% and 80% of stilbene in polystyrene matrix highlighting amorphous peaks which corresponds to the distance of interchain ordering

These results highlight a hidden structural response of the amorphous phase, often masked by intense crystalline peaks in XRD patterns. The study emphasizes that molecular crystallization in polymer composites is accompanied by significant modifications of the surrounding amorphous environment, which should be considered when interpreting diffraction data and structure–property relationships in organic functional materials.

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Molecular Dynamics-Based Structural Sampling: Case Studies of Stilbene, Urea, and Carotenoid Complexes

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Hydrogen bonding plays an important role in nature, from carotenoids and stilbenes to urea [1-6]. Carotenoids are responsible for the coloration of leaves, fruits, flowers, and other organisms, and they play a critical role in photosynthesis through light-harvesting and photoprotective functions. In these processes, hydrogen bonding can be significant, which motivates the need to understand the effects of polar solvents [2−4]. Stilbenes are diarylethenes that exhibit fluorescence and reversible photoisomerization upon UV excitation. The influence of the environment, such as polystyrene, on stilbene geometry remains an open question [5]. Urea is an efficient hydrogen-bond donor and acceptor, making it a suitable model compound for studying polar interactions [6].

A polar environment can induce new molecular arrangements, and molecular dynamics (MD) is a suitable tool for exploring such structural diversity. In this work, we show how stilbene-based complexes are formed, discuss the challenges of obtaining stable complexes in a realistic urea solvent, and finally present possible new complexes involving carotenoids - with particular emphasis on fucoxanthin - in protic and aprotic polar solvents.

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