

DOC 2020 16th INTERNATIONAL YOUNG SCIENTIST CONFERENCE

ABSTRACT BOOK









16th International Young Scientist conference

Developments in Optics and

Communications 2020

Dear participants of DOC 2020,

The **DOC** conference is organized jointly by University of Latvia SPIE student chapter, OSA Latvian student chapter and University of Latvia. The purpose of this conference is to bring together students and young scientists working experimentally and theoretically in the fields of optics and photonics to share and exchange new ideas and to establish contacts for future collaboration.

Unfortunately, the face to face events of **DOC 2020** were canceled due to the pandemic. However, both we the organizers and you the participants have invested a lot of our time For **DOC 2020**, the event were planned behind the scenes, research was done, abstracts written, reviewed and accepted. We have prepared this abstract book to preserve all fo our hard work.

Best regards, DOC 2020 Organizers

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Invited Speakers

Biophotonics in Microcirculation Imaging

Martin Leahy

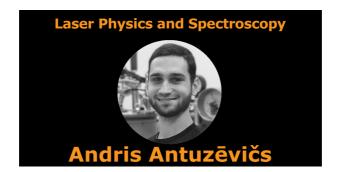
 $National\ Biophotonics\ and\ Imaging\ Platform\ Ireland,\ National\ University\ of\ Ireland,\\ Galway$



Electron magnetic resonance in optical materials

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Electron paramagnetic resonance (EPR) spectroscopy encompasses a set of techniques, which are valuable for the investigations of materials possessing unpaired electrons. In this talk general aspects of EPR spectroscopy will be explained with a focus on applications in optical materials. Examples will be given on the characterization of luminescent glass ceramics, photochromic materials, X-ray radiation colored glasses and functional materials relevant to fusion reactors. Main principles of optical detection of magnetic resonance will also be covered.

Non-luminescent defects in phosphors: tailoring the material

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Phosphorescent materials are able to store excitational energy in the crystal lattice and emit it in the form of light minutes or even hours after the termination of excitation. Many applications have been found for this class of materials in geological dating, safety inks, mechanoluminescent detectors, dosimeters and others [1]. Rare earth ions play a very important role in these materials - they can contribute both as luminescence centers as well as influence the emission and excitation behaviour by modifying the trapping centers in the materials [1,2]. What is interesting is that for many materials the exact nature of the defects contributing to the storage and release of the excitational energy is not known. Advanced analytical methods combined with theoretical calculations can be used to help solve these puzzles, but that is yet to be done.

Different types of defects in the phosphorescent materials can interact with each other and the host material lattice therefore influencing the storage and release conditions. Those defects may help to tailor the materials for our needs - if we want the release of light to happen under special circumstances (light, heat, pressure, radiation) or for a definite amount of time, we are able to design the material for our needs.

- [1] V.Vitola, D. Millers, I. Bite, K. Smits & A. Spustaka, Recent progress in understanding the persistent luminescence in SrAl2O4:Eu,Dy, Materials Science and Technology (2019), 1661-1677
- [2] J. Xu, S. Tanabe, Persistent luminescence instead of phosphorescence: History, mechanism, and perspective. J Lumin. 2019;205:581–620.

From stars to the eye. Adaptive Optics applications for Visual Optics

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The eye is an optical instrument that project scenes of the visual world onto the retina. However the human eye is far from being a perfect optical system, and, as a consequence, the images projected on the retina are blurred by ocular aberrations, as well as diffraction and scattering. Therefore in the last years, multiple technologies based on wavefront sensing and Adaptive Optics (AO) have been developed for the measurement and correction of ocular aberrations. As a result important knowledge has been gained on the contribution of the different components of the eye to the degradation of image quality. However the processes underlying neural adaptation to ocular aberrations are not yet well understood.

Typically, the impact of ocular aberrations on vision is studied using wavefront sensors with monochromatic, generally infrared, light. However, the retinal image quality is degraded by the presence of both monochromatic and polychromatic aberrations in the ocular optics. The study of the impact of retinal image quality on vision should therefore consider both the aberrations in the visible light, as well as the effect of chromatic aberrations. In addition optical and structural properties of the eye change with age and with certain ocular conditions and treatments, altering the natural aberrations, as well as the interactions between monochromatic and chromatic aberrations, and consequently the visual function. The understanding of the interactions of these aberrations and their effect upon correction is essential to explore the limits of human spatial vision, and to design and optimize new alternatives of correction of Presbyopia/Myopia and more complex individualized refractive corrections.

Moreover, AO-based visual simulators have allowed the simulation of new optical solutions to optically correct for Presbyopia, the age-related loss of the accommodative amplitude of the human eye, and to explore the effect of multifocal simultaneous vision corrections with different designs on vision, in the presence and absence of natural aberrations.

Part I Biophotonics

Development of New Optical Immunosensors Based on Photoluminescence TiO2 nanostructures

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Immunosensors based on hybrid metal oxide nanostructures (TiO2, ZnO, WO3, etc.) are broadly applied in different spheres of human life – from medical diagnostics up to national security and defense [1,2]. Immunosensors are based on a specific interaction between the antibody – antigen couple which has high specificity and sensitivity to detect analytes [3]. Optical immunosensors, are increasingly studied class of biosensors because they allow the evaluation of some inter-molecular interactions contactless, without the damage of biological samples and without chemical or physical labels [3]. Therefore, development of biosensors based on the optical detection methods that can be applied for the determination of large variety of analytes is of great interest.

Among many different immunosensors, the photoluminescence-based sensors seem to be the most promising for the improvement in the diagnosis of virus induced diseases. In photoluminescence-based immunosensors, the nanostructured metal oxides such as ZnO or TiO2 are often used as very efficient photoluminescence transducers [1,3,4]. TiO2 and its hetero-structures are extensively used as wide-band gap semiconductors with a unique combination of physical and chemical properties [2]. A good biocompatibility of TiO2 nanostructures, their applicability at pHs in the range of 5.5–7.0 and high chemical stability have resulted in the extensive application of TiO2 in electrochemical [2], electrical [5] and optical biosensors [2,3]. In the range of optical biosensors the changes in the photoluminescence spectra were exploited as analytical signal for the determination of target analyte [1,3,4]. However, the interaction mechanism of proteins with TiO2 and the origin of the changes in the photoluminescence spectra were poorly discussed, although the mechanism of the interaction between semiconductor and proteins is the key in solving many of problems, which are still arising during the development of TiO2-based immunosensors, such as an improvement of sensitivity and selectivity [1,6]. This work is aiming to highlight the origin of the changes in the photoluminescence spectra of TiO2 resulted after the protein adsorption on its surface during the formation of biosensitive layer and after its interaction with target analyte. In this research, Bovine leukemia virus protein gp51 was applied in the design of photoluminescence-based immunosensor. As it is proposed, the main reason of the shifts of photoluminescence signal observed after modification of TiO2 by gp51 proteins is based on electrostatic interaction between partial charges of adsorbed gp51 protein and negatively charged TiO2 surface.

- [1] A. Tereshchenko, M. Bechelany, R. Viter, et.al., Sensors and Actuators B, Chemical 229, 664 (2016).
- [2] S. Ramanavicius, A. Tereshchenko, R. Karpicz, et.al., Sensors, 20, 74 (2020)
- [3] A. Tereshchenko, V. Fedorenko, V. Smyntyna, et.al., Biosensors and Bioelectronics 92, 763 (2017).

- [4] R. Viter, A. Tereshchenko, V. Smyntyna, et.al., Sensors and Actuators B: Chemical, 252, 95 (2017)
- [5] Y.-M. Chu, C.-C. Lin, H.-C. Chang, et.al., Biosensors and Bioelectronics, 26, 2334 (2011).
- [6] A. Tereshchenko, V. Smyntyna and A. Ramanavicius, RSC Advances, 8, 37740 (2018)

Development of the multimodal laser device for skin diagnostics

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In the Institute of Atomic Physics and Spectroscopy we have developed multimodal skin diagnostic prototype device. It is a simple and easy-to-use tool for dermatologists and also can be used for scientific institutions and laboratories. Device is intended for optical diagnosis of the skin lesions (melanoma, vascular formations, burn injuries etc.). It can be used in dermatology, oncology, cosmetic, surgery, trauma, burns treatment etc. Used optical technologies are non-invasive, patient friendly and informative, with diagnostic potential. Device captures several multimodal images from the skin pathology area, and extracts clinically significant information [1]. The device software algorithm also calculates skin chromophore (haemoglobin, melanin) relative concentration maps. The results are shown on the 4.3 inch screen with touch. Device is based on Windows CE 7.0 operating system. Device has in build processing software for near real-time calculation of skin chromophores and parameters. One measurement procedure takes only 4 seconds [2]. The skin is illuminated by five wavelength low power (40mW) lasers that are arranged in a ring around the camera lens. In total, 20 lasers are operated – sets of 4 emitting at five various wavelength bands (peaks at 405, 450, 520, 660, and 850 nm), and 4 white LEDs for preview mode. Each set of equal lasers is powered separately by a constant current laser driver. The LED radiant spectral half-width 25 nm, while the lasers radiate in a much narrow spectral band 2 nm. The narrow spectrum of the lasers is an advantage of this device, since only specific skin chromophores are excited when the skin is radiated with narrower spectrum radiation. This is an important factor in image processing and directly influences the accuracy of the calculated result. A system on chip module Nvidia Tegra 2 T20 with a 1 GHz dual core ARM Cortex-A9 processor is used as a central processing unit. It provides smooth operation of all the device's internal components and GUI. A 3 Mpix RGB CMOS matrix with 3.2-µm size pixels serves as the image sensor, and it is connected to a central processor via a 10-bit parallel line. A removable SD memory card stores captured images. Installing and updating devices software is possible trough mini USB connector. By removing the SD memory card calculations of parametric maps can be performed in PC [3].

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- [1] I.Oshina, J.Spigulis, U.Rubins, E.Kviesis-Kipge, K.Lauberts, "Express RGB mapping of three to five skin chromophores", Proc. SPIE-OSA 10413, 104130M-1 (2017).
- [2] E. Kviesis-Kipge, U. Rubīns, O.Rubenis "Multimodal imaging device for skin diagnostics: improvements and tests". DOI: 10.1109/BEC.2018.8600952, (2018) https://ieeexplore.ieee.org/[3] J.Spigulis. "In vivo skin imaging prototypes "made in Latvia"", Front. Optoelectron.,

1-12, https://doi.org/10.1007/s12200-017-0717-5 (2017).

Luminescence of AlN:Mn powders

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AlN is a perspective material for studying biological processes due to its low toxicity and overall inertness. In addition, the long-lasting luminescence caused by manganese impurities at 600 nm may be particularly relevant in the research of living organisms because of high transmittance of red and infrared light through tissue in this spectral region.

Luminescence of AlN:Mn macro- and nano-size powders was studied using material spectral characterization including measurement of photoluminescence and its excitation spectra as well as luminescence kinetics in various environments and temperatures. The well-known Mn-caused red luminescence peaking at 600 nm appeared being dominant in all materials. It was observed that there are two spectral regions where the red luminescence can be excited, forming wide and complex excitation bands peaking at 520 nm and 260 nm. It was also found that excitation of AlN:Mn at both spectral regions around 520 nm and 260 nm PLE results in long-lasting luminescence.

Analysis of experimental results and their comparison with those obtained in undoped AlN materials allow the conclusion that there are two defect-caused mechanisms originating Mn luminescence. One of them is the so-called intra-center mechanism, but other is recombination mechanism realizing at 520 and 260 nm excitations, respectively.

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Part II Laser physics and spectroscopy

Density of quantum states in periodical structures

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New quantum effects have been studied in thin nanograting layers. Nanograting on the surface imposes additional boundary conditions on the electron wave function and reduces the density of states. When the dimensions of the nanograting are close to the De Broglie wavelength the density of states reduction is considerable and leads to change in the layer properties. Calculations of the density of states are challenging to perform and are related to the quantum billiard problem. Performing such calculations requires to find solutions for the time-independent Schrodinger equation with Dirichlet boundary conditions [1]. It was one of the goals of this work to solve this problem using numerical methods. There is a full mathematical analogy between quantum billiards and electromagnetic resonators. Therefore, it is reasonable to use the Method of Auxiliary Sources (MAS) for quantum billiard calculation, as it is most efficient numerical approach for solving eigen value problems. It was one of the goals of the project to solve this problem using digital methods. MAS has been proposed by Georgian mathematician V. Kupradze [2]. Method was adopted by Georgian scientists for solving eigen value problems related to wave guides with arbitrary cross-section [3, 4]. In the MAS for EM boundary value problems are solved numerically by representing the electromagnetic fields in each domain of the structure by a finite linear combination of fundamental solutions of the relevant field equations, corresponding to sources situated at some distance from the boundaries of each domain. The "auxiliary sources" producing these solutions are chosen to be elementary currents/charges located on fictitious auxiliary surface, usually conforming to the actual surface of the structure. The method only requires points on the auxiliary and actual surfaces, without resorting to the detailed mesh structures as required by other methods. Finally the problem is reduced to linear system of algebraic equations which solutions are coefficients of the decomposition. Coefficients should be obtained by solving of the mentioned linear system where one of the coefficients is fixed. It means that the field inside area of interest becomes non-trivial only when the main parameter of the problem is near to eigenvalues and we can easily observe the forming of eigenfunctions. Intensity of the field reaches maximum on eigenvalues. The calculations are performed in Fortran.

- [1] N. Peranio, M. Winkler, D. Bessas, Z. Aabdin, J. König, H. Böttner, R.P. Hermann, O. Eibl, Journal of Alloys and Compounds, 521, pp. 163–173, 25, (2012).
- [2] A. Tavkhelidze, V. Svanidze, International Journal of Nanoscience, Vol. 7, No. 6, pp. 333-338, (2008).
- [3] A. Tavkhelidze, J. Appl. Phys. 108, 044313 (2010).
- [4] V. Kupradze, in Success of Mathematical Sciences, vol. 22, Moscow, 1967, pp. 59-107

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Theoretical insights into the electronic structure and low-lying states of the RaCl molecule promising for laser cooling

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The applications of ultracold molecules include ultra-high-resolution spectroscopy, few-body physics, quantum computation, molecular optics and controlled chemical processes [1]. Earlier [2] it was shown that diatomic molecules, which contain alkaline earth metal atom and halogen atom are promising for the direct laser cooling due to the matching equilibrium internuclear distances for different potential energy curves (PECs).

In this study, *ab initio* state-of-art calculations of the low-lying states of the RaCl molecule were performed for the first time.

The calculations at the SA-CASSCF(13,12)/XMCQDPT2 + SOC [3] level of theory were carried out including spin-orbit coupling (SOC). The TZ-basis set for Cl atom and Stuttgart RSC ECP 78 for Ra atom were used in the calculations for three dissociation limits $[Ra(7s^2)+Cl(3p^5), (Ra^+(7s)+Cl^-(3p^6), and Ra^+(6d)+Cl^-(3p^6)].$

The PECs and spectroscopic parameters were obtained for the ground and eight excited RaCl $(n)\Omega$ terms. It is shown that the ground and five first excited states have an ionic character in the region of PECs minima. Based on the calculations of the vibrational energies and the Franck-Condon factors, we conclude that the radium chloride molecule is a promising candidate for the direct laser cooling.

- [1] O. Dulieu, C. Gabbanini. Rep. Prog. Phys. 72, 086401 (2009).
- [2] T.A. Isaev, S. Hoekstra, R. Berger. Phys. Rev. A 82, 052521 (2010).
- [3] A.A. Granovsky. J. Chem. Phys. 134, 214113 (2011).

Computational and experimental studies on structural and spectral properties of some diphenoxyadamantane alkylamine derivative

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Adamantane derivatives are objects of intense studies in the fields of medicinal chemistry and drug design due to their particular biological activities. Due to high antiviral activity some adamantane derivatives are used as drugs against Influenza A virus and HIV. These derivatives also possess anticancer, antimicrobial, antifungal and anti-inflammatory activities [1]. Pharmacologically active drugs usually have complex structure with a wide spectrum of structural conformers. This aspect makes difficult a prediction and interpretation of important spectral properties of such compounds.

In this study we perform the results of comprehensive research on structural and spectral properties (IR, Raman and UV/Vis spectra) of adamantane-containing compound: 2,2',2",2"'-(((2S,2'S)-(((1S,3S,5S,7S)-adamantane-2,2-diylbis (cyclohexane-4,1-diyl)) bis (oxy))bis(2-hydroxypropane-3,1-diyl))bis(azanetriyl))tetraethanol dihydrochloride. First of all, the conformer search procedure was done. Based on the structure of the compound and our chemical intuition ten dihedral angles were chosen, the changes of which generate main conformers. Search for conformers and geometry optimization of the structures was carried out by the DFT approximation (B3LYP/cc-pVDZ). We found four the most stable conformers with relative energies of 0.0, 1.5, 6.4 and 6.5 kcal/mol.

The FT-IR (reflection mode) and Raman scattering spectra of the compound for the crystalline phase were measured in the ranges of 4000-400 and 3200-150 cm⁻¹, respectively. The experimental measurements were followed by quantum-chemical calculations for prediction of the vibrational IR and Raman spectra for all conformers at the B3LYP/cc-pVDZ level of theory in the harmonic approximation. The UV/Vis spectrum of solution of the compound in ethanol was measured in the range of 450-200 nm. The spectrum registered is complicated, consisting of several broad absorption bands. For interpreting the spectrum obtained the calculations at the Time-Dependent DFT and Multi-Reference Perturbation Theory levels of theory were carried out for all the conformers. The compound comprises several functional groups. This fact leads to arising of the intramolecular charge transfer that courses the difference in the results of the calculations by two different approximations, showing the inapplicability of TDDFT approach.

This work was supported by Belarusian Republican Foundation for Fundamental Research (project No. F18MS-046).

References

[1] G. Ali Mansoori, P.L. Barros de Araujo, E. Silvano de Araujo, *Diamondoid Molecules* (World Scientific Publishing, Hackensack 2012)

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Whispering gallery mode microresonator as a humidity sensor

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Whispering gallery mode microresonators (WGM) are widely researched due to their high quality (Q) factors and sensitivity. High Q factor is the result of the structure of the resonator: microspheres, microbottles, and other cavities that have smooth edges and are transparent, with refractive index higher than that of surrounding environment. Therefore continuous total internal reflection occurs [1]. There are many applications to WGM microresonators, such as spectroscopy and fluorescence studies, generation of frequency combs, biosensing and many others [2]. This study explores WGM microresonator as a humidity sensor, using glycerol microsphere.

Precise humidity measurements are important in various sectors: industrial processing, environmental control, automobile industry, medical field, agriculture, and general industry [3]. However, the available humidity sensors can be slow and not work in low/high humidity. This study researches the precise measurements of relative humidity (RH), using a silica microsphere dipped in pure glycerol and a tunable laser. For the experiment, glycerol was chosen due to its hygroscopicity, transparency and its stability in time and temperature. As glycerol absorbs water, its radius and refractive index change, resulting in a shift in resonant wavelength An integer number of wavelengths fit the optical path of the resonator [4]. To obtain whispering gallery resonances tunable laser with wavelength 760 nm was used. Light from the laser excites the microsphere and shift in resonant frequencies was observed using an oscilloscope.

Glycerol as a resonator is stable both in time and temperature, with fast reaction time, and it works in all ranges of RH. Using an oscilloscope, data was collected in the range from 55 to 65 % RH, shift in modes was observed. The results of this experiment show that glycerol droplet as a RH sensor is very precise, which is necessary for many industrial needs and scientific studies. Further research on this subject is necessary to test the resonator in low humidity levels, as well as test the repeatability and hysteresis of this sensor.

This study was financed by LZP project Nr.lzp-2018/1-0510 'Whispering gallery mode microresonator sensors'.

- [1] X. Jiang et al., Whispering gallery microsensors: a review, Cornell University, arXiv:1805.00062 (2018).
- [2] M. Gomilsek, Whispering gallery modes, University of Ljubljana (2011).
- [3] Z. Chen, C. Lu, Humidity Sensors: A Review of Materials and Mechanisms, Sensor Letters 3, 274-295 (2005).
- [4] L. Labrador-Paez et al., Liquid whispering-gallery-mode resonator as a humidity sensor, Optics Express 25, 1165-1172 (2017).

Ab initio calculations of the low-lying states of the KFr molecule

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Ultracold (<1 mK) polar diatomic molecules (atomic dimers), which include atoms of various alkali metals, are the subject of intense experimental and theoretical studies. Ultracold molecules offer promising applications such as new platforms for quantum computing, precise control of molecular dynamics, nanolithography and Bose-enhanced chemistry [1]. For the applications mentioned one needs to produce such molecules in the absolute ground state with zero values of vibrational and rotational quantum numbers. So the knowledge about the ground and low-lying electronic states, spectral and other properties of ultracold diatomic molecules are crucial for potential use, which can be obtained by series of experiments or by performing ab initio quantum-chemical calculations and applying appropriate molecular theories.

The diatomic polar KFr molecule is an example of the above-mentioned compounds. The francium does not have stable isotopes; the longest-lived isotope of francium is 212 Fr with a half-life of about 20 minutes. It is the main restraining factor for using francium atom in a laser-cooling experiment. To the best of our knowledge, there are not any calculations of the electronic states of the francium-containing diatomics at the high level of theory.

The main goal of this study is the prediction of the potential energy curves (PECs) of the ground and some excited states of the KFr molecule. In this work, the SA-CASSCF(2,8)/XMCQDPT2 [2] calculations of the low-lying singlet and triplet states of the KFr molecule were performed. The Stuttgart RSC effective core potentials and corresponding TZ-basis sets were used for the K and Fr atoms. The calculations were performed pointwisely by steps of 0.2, 0.25, and 1.00 Å for the internuclear distances ranging 3.6-4.2, 4.2-10.0, and 10.0-16.0 Å, respectively. To obtain more reliable energies the XMCQDPT2 method [2] was used. All the 8 lowest double occupied orbitals were involved in the perturbation calculations. The dimensions of the effective Hamiltonian were 30×30 and 28×28 for the singlets and triplets, respectively. We obtained PECs for 8 singlet and 10 triplet terms. The results of our calculations of the spectroscopic parameters of the KFr ground state $X^1\Sigma^+$ are following: Re = 4.230 Å, De = 3659 cm⁻¹. For the excited states we also obtained all spectroscopic molecular parameters.

- [1] L.D. Carr, D. DeMille, R.V. Krems, J. Ye. New J. Phys. 11 (2009) 055049.
- [2] A.A. Granovsky. J. Chem. Phys. 134 (2011) 214113.

Ab initio multi-reference perturbation theory study on the LiFr molecule

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Nowadays, the study of cold and ultracold polar molecules is one of the most promising research directions. This is mainly due to that cold and ultracold polar molecules offer prospects for the realization of a new form of quantum matter (Bose-Einstein condensate) [1]. One of the possibilities of obtaining molecular quantum matter with controlled properties is the transferring of the polar diatomic molecules to the ground rovibronic state by initial optical excitation into the overlying rovibronic states with specific forms of electronic terms. In this case for the high efficiency of excitation and subsequent relaxation of the molecular system, it is required knowledge of the exact forms of the potential energy curves (PECs) of the combining electronic states. The construction of exact empirical terms is performed based on of the analysis and interpretation of high-resolution rovibronic spectra and may be based on ab initio potential curves. The knowledge of the exact PECs also allows defining the important spectra-energetic characteristics of molecules and the macroscopic physical properties of rarefied gases.

The diatomic polar LiFr molecule is an example of the above-mentioned compounds. The francium does not have stable isotopes; the longest-lived isotope of francium is ²¹²Fr with a half-life of about 20 minutes. It is the main restraining factor for using francium atom in a laser-cooling experiment. To the best of our knowledge, there are not any calculations of the electronic states of the francium-containing diatomics at the high level of theory.

In this study, the SA-CASSCF(2,10)/XMCQDPT2 calculations of the low-lying singlet and triplet states of the LiFr molecule were performed. The calculations were carried out in two stages (the CASSCF and the XMCQDPT2 [2] levels of theory) in a wide range of internuclear distances. The TZ-basis set for Li atom and Stuttgart RSC ECP78MDF (for Fr atom) have been used in calculations. We obtained PECs for 9 singlet and 8 triplet terms. The results of our calculations of the spectroscopic parameters of the LiFr ground state $X^1\Sigma^+$ are the following: $R_e=3.681$ Å, $D_e=5145.62$ cm⁻¹. For the excited states, we also obtained all spectroscopic molecular parameters.

Based on the obtained data, the calculation of the main transport properties will be carried out for LiFr molecule, as well as the refinement of the form of the term curves taking into account symmetry.

- [1] L.D. Carr, D. DeMille, R.V. Krems, J. Ye. New J. Phys. 11 (2009) 055049.
- [2] A.A. Granovsky. J. Chem. Phys. 134 (2011) 214113.

Calculation of the 2D PES for the molecules of common formula xyzyx: importance of a symmetry accounting

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It is well known that sometimes the specific class of molecules can be represented by the common structural formula. For example polyoxides can be specified as $\mathrm{HO}_n\mathrm{H}$, were n- is a number of the oxygen atoms. Cremer [1] was the first who has proposed to consider HOOOH as a prototype molecule for geminal double rotors. Now it is obvious that the wider group of molecules can be specified by the common formula XYZYX, where X=H, D, F..., Y=O, S, Z=CH₂, O, S. All of these molecules with geminal double rotors have a common properties. They have two equilibrium configurations – transand cis- conformers. The first one belongs to C₂ and the second one belongs to C₅ point groups of symmetry. Tunneling between two equivalent configurations in both conformers is possible for all molecules too. Finally, all conformers and configurations of all molecules can be described by $\mathrm{C}_{2V}(\mathrm{M})$ group of molecular symmetry. According to symmetry analysis performed in [2,3] 2D PES of all XYZYX molecules has four triangles, all points of which are connected by symmetry operations as it is shown in Fig.1.

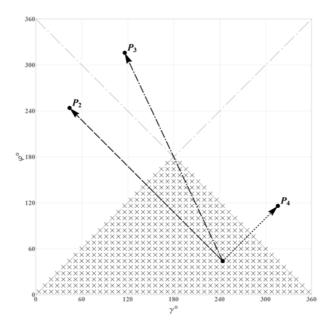


Figure 1: The equivalent points generated by symmetry operations of the $C_{2V}(M)$ molecular symmetry group.

As it is seen from Fig.1 symmetry elements P_2 and P_4 are symmetry planes while P_3 is the center of inversion. As it was shown in [3] correct accounting of the symmetry properties is very important for precision calculations of the tunneling frequencies. In this work we represent a few methods of preparation of calculated data and compare the results obtained values of tunneling frequencies for the trans- and cis- conformers of the analyzed molecules.

- [1] D. Cremer, J.Chem.Phys., 69 (1978) 4456-4471
- [2] G.A. Pitsevich, A.E. Malevich, U.U. Sapeshka, J.Mol.Spectr., 360 (2019) 31-38
- [3] G.A. Pitsevich, A.E. Malevich, U.U. Sapeshka, Chem. Phys., 530 (2020) 110633

COMPARISON OF THE BARRIERS TO INTERNAL ROTATION IN THE HOCH2OH, HOOOH, HOSOH AND HSSSH MOLECULES

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Internal rotation in the molecules as well as torsional vibrations have been attracting the attention of the researchers for a long time. Nature of the potential barriers to internal rotation and the shape of the potential energy surface (PES) are the subjects of many investigations. Not so long ago [1,2] we analyzed the properties of the 2D PES and symmetry of the torsional vibrations in the HOCH₂OH and HOOOH molecules. Recently we performed similar calculations for the HOSOH and HSSSH molecules. All these molecules belong to $C_2V(M)$ molecular symmetry group and due to this have the similar but not the identical 2D PES (see, for example, 2D PES of the HOCH₂OH and HSSSH in Fig.1).

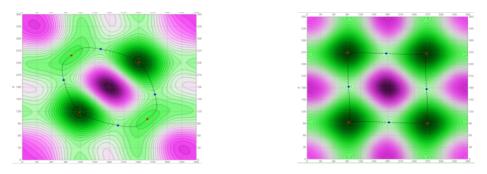


Figure 1: 2D PES and minimum energy paths from the global to the local minimums in the HOCH₂OH (left) and HSSSH (right) molecules.

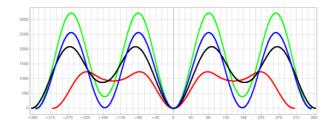


Figure 2: arriers to internal rotation along the minimum energy path in the HOCH₂OH (red), HOOOH (black), HOSOH (green) and HSSSH (blue) molecules.

Processing the calculation results allows us to combine in one figure (see Fig.2) potential barriers to internal rotation for the all four analyzed molecules.

Fig.2 lets us understand more clearly the possibility of a) existence of the cis-conformers of the studied molecules as well as b) tunneling of the hydroxyl or thiol groups.

- [1] G.A. Pitsevich, A.E. Malevich, U.U. Sapeshka, J.Mol.Spectr., 360 (2019) 31-38.
- [2] G.A. Pitsevich, A.E. Malevich, U.U. Sapeshka, Chem. Phys., 530 (2020) 110633

PMMA WGM microsphere resonator quality factor measurements using video recodnition, temperature changes and fixed wavelenght

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The whispering gallery modes (WGM) resonators are based on spherical objects, which are made from optically transparent materials, and is capable of maintaining an circling optical wave, inside the sphere, using total internal reflection. If there is a light source which supply the sphere with constant intensity, the wave moving along the perimeter of sphere starts constructively interfere. In this case the resonance happens, which is called whispering gallery mode (WGM). When there is a change in temperature, it changes the radius of WGM resonator, and that results in change of reflection coefficient, which results in change of resonance and intensity. The current work explores the possibility of using temperature changes to measure polymethyl methacrylate (PMMA) WGM microsphere resonator quality factor (Q) and thermal expansion parameters. Different diameter and material spheres are used in the experiments for equipment testing and calibrating. The two main parameters which determine the WGM microresonator resonance peak change with temperature are the linear thermal expansion coefficient α and the optical index of refraction change with temperature β (thermorefractive coefficient) which also changes with the wavelength of used light In our measurements we have a simplified case where laser wavelength is constant and resonance tuning is induced by changing temperature. From the obtained traces peak width and repetition free spectral rage was measured manually and Q-factors were calculated for several different size PMMA micro resonators Our result show that thermal coefficient slightly increases for smaller resonators probably. For best results of thermal coefficient, would, be if the WGM micro resonator size would be around $130-140\mu m$, where the results come close to their bulk material value of 80*10-6/K[1]. The performed experiments show a very simplified way of measuring Q-factors for WGM micro resonators and determining thermal coefficient. This opens up a window for new measuring tool and method deign, that would be very useful for people working with WGM resonators [2]

- [1] Z. Zhang, P. Zhao, P. Lin, F. Sun, Thermo-optic coefficients of polymers for optical waveguide applications, Polymer 47, 4893 (2006).
- [2] A. B. Petermann, A. Varkentin, B. Roth, U. Morgner, M. Meinhardt-Wollweber, All-polymer whispering gallery mode sensor system, Optics Express 6, 6052 (2016).

Computer simulation of the effects of added zinc oxide nanolayer to wgm microresonators

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The WGM (whispering gallery mode) microresonators are spherical or cylindrical optical structures where light can "rotate" inside due to total internal reflection. When an integer number of light waves fits into the perimeter of the microresonator, constructive interference takes place and resonance occurs [1]. The quality factors of WGM microresonators are very high - around 10⁶, so the resonant frequency is narrow, which is good for using a laser and having a precise measurement. The WGM microresonators are sometimes called the morphologically dependent resonators [2] because the resonant frequency is dependent on the form of the microresonator. Small changes in the environment are picked up by microresonators changing their radius or refractive index, thus changing the resonant frequency. This allows WGM microresonators to be used as sensors. Sometimes it's good to coat the microresonator with an extra layer, for example, a zinc oxide layer. This layer helps to later stick antigens for biosensing. The effects of adding this extra layer can be simulated using COMSOL Multiphysics software. The extra layer changes how close to the surface the light is propagating and ads extra modes. Various methods are used for exploration of this topic such as using random functions to better describe the roughness of the surface, witch in micro and nanoscale makes a difference.

- [1] Chiasera, A., Dumeige, Y., and Patrice, F. (2010). Spherical whispering-gallery-mode microresonators. 482(3), 457–482.
- [2] Yang, S., Wang, Y., and Sun, H. D. (2015). Advances and Prospects for Whispering Gallery Mode Microcavities. Advanced Optical Materials, 3(9), 1136–1162.

THIOL GROUPS TORSIONAL VIBRATIONS IN THE HSSSH MOLECULE

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Thiols is an interesting class of molecules containing S-H group. They find a lot of applications in different areas of chemistry. Trisulfane (HSSSH) molecule is a second member of the following group of molecules HS_nH (n=1,2,3..). Structure and internal rotation in the hydrogen disulfide (HSSH) molecule was intensively studied and often compare with the same properties of hydrogen peroxide (HOOH) molecule. It is actually interesting to understand how substitution of the oxygen to sulfur atom changes 1D PES associated with internal rotation in these molecules. Recently [1] we analyzed the 2D PES and torsional vibrations in the hydrogen trioxide molecule (HOOOH). It is obviously interesting to compare 2D PES and peculiarity of the torsional vibrations in the HOOOH and HSSSH molecules. As far as we know the 2D PES and tunneling in the ground state of the trisulfane molecule was investigated only in [2]. However, details of this calculations as well as energies of the stationary torsional levels are absent in this work.

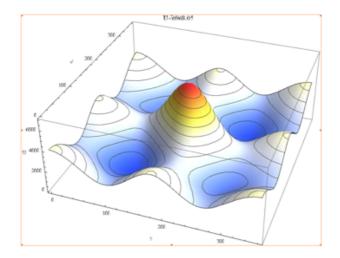


Figure 1: 2D PES of the HSSSH molecule calculated at the CCSD(T)acc-pVTZ level of theory.

In this work, we performed the calculations of the 2D PES (see Fig.1) and energies of the torsional levels at the CCSD(T)/acc-pVTZ level of theory. The calculated values of the torsional states energies are presented in Tabl.1.

Based on calculated data the low-temperature torsional spectra of the ${\it HSSSH}$ molecule were predicted too.

1	2	3		4	5	6				
	рооон									
Energy level number	Conformation	Energy [cm ⁻¹]	Energy splitting [cm ⁻¹]	n_{sym}	n _{asym}	Symmetry species				
1	trans	0	4 manuall	0	0	$A_{1} + A_{2}$				
2	trans	1.73*10-11	1.73*10 ⁻¹¹	0	0	$A_1 + A_2$ $A_1 - A_2$				
3	cis	23.018	1.97*10-11	0	0	$A_{\rm l}$				
4	cis	23.018	1.9/*10	0	0	B_2				
5	trans	293.575	4.51010:11	1	0	$A_{\rm l}$				
6	trans	293.575	4.51*10-11	1	0	A_2				
7	trans	317.616	2.20*10:10	0	1	B_1				
8	trans	317.616	2.39*10-10	0	1	B_2				
9	cis	327.102	2 40#10:10	0	1	$B_{_{1}}$				
10	cis	327.102	2.49*10 ⁻¹⁰	0	1	A_2				
11	trans	341.362	2.14#10:10	1	0	$A_{\rm l}$				
12	trans	341.362	2.14*10 ⁻¹⁰	1	0	В,				

Table 1: The calculated at the CCSD(T)acc-pVTZ level of theory values of torsional states energies of the HSSSH molecule and their assignments.

- [1] G.A. Pitsevich, A.E. Malevich, U.U. Sapeshka, Chem. Phys., 530 (2020) 110633
- [2] C. Fábri, Ĺ. Horný, M. Quack, ChemPhysChem 16 (2015) 3584-3589

Tops torsional vibrations in methyl hydroperoxide

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The studies of 2D Hamiltonian model based on two torsional tops and spreaded to full 15D dimentionality for the probing seven-atoms molecule of methyl hydroperoxide by the use of TNum package [1] revealed multi-dimentionality effect (MDE) on the kinetic energy operator parameters [2].

The present work is to continue the investigation by involving into research the full energy of the probing system through a calculation of its frequencies resulted from the torsional vibrations as an object of both the model monitoring and the practical use in spectroscopic applications and polimerization reactions.

As a start point, one uses the 2D geometry on the multi-dimentionality scale, and Figure 1 shows configuration of all the seven atoms.

To set up torsional states for the denote starting configuration, one uses also free of charge package known as GAMESS [3] to derive the frequencies from the full energy simulation. Table presented shows simulated values in comparison with the literature data. The difference observed between values of harmonic and anharmonic fre-



Figure 1: Space locations of methyl hydroperoxide atoms used as start geometry for the MHP molecule tops.

quencies comes from taking into account anharmonic corrections based on invoking correlating effects calculated by the use of the method of vibrational self-consistent field [4]. In general, we hope that the results obtained help to throw light on the discussion concerning the MDE revealed [2,5].

Table 1: MHP harmonic (2, 3, 4 columns) and anharmonic (5, 6, 7 columns) frequencies

	ν , cm ⁻¹					
	[PW]	[6]	[7]	[PW]	[PW]	[6]
Method	MP2	VPT2	MP2	MP2	MP2	MP2
	/cc-pVDZ		/6-31G	/cc-pVDZ	/PT2-VSCF	/cc-pVTZ
				/VSCF	/cc-pVDZ	
OH-top	170	200	165	124	124	127
CH3-top	273	254	267	262	262	250

References

- [1] D. Lauvergnat, A. Nauts, J. Chem. Phys., **116**, 8560–8570 (2002)
- [2] Y. Zubrytski, DOC Riga 2019 Books of Abstracts, 59 (2019)
- [3] M. W. Schmidt et. al., J. Comput. Chem., 14, 1347–1363 (1993)
- [4] C. A. Brindle, Phys. Chem. Chem. Phys.,

textbf7, 945-954 (2002)

[5] Y. Zubrytski, Numerical Modeling of Internal Rotation and Calculation of Torsional

Frequencies in Methyl Hydroperoxide, (Master Thesis, BSU, Miensk, 2019)

- [6] S. Dalbouha, M. L. Senent, and N. Komiha, J. Chem. Phys., 142, 074304-1-9 (2015)
- [7] M. Tyblewski, J. Chem. Phys., **97**, 6168–6180 (1992)

New spectroscopic data on the $c^3\Sigma^+$ state of KCs

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Accurate empirical data on excited electronic states manifold in alkali diatomics containing heavy alkali atom, such as Cs, are necessary in order to predict convenient optical paths for creation the ultracold (below 1 mK) diatomic species from the respective ultracold atomic pairs. Regarding KCs, the interest is connected with the possibility to apply the short-range photoassociation via the $B^1\Pi$ state [1,2], which becomes possible due to its interaction with the near lying states of triplet character, to the largest extent by the first excited electronic triplet $c^3\Sigma^+$ state. The latter was first studied in [3], but the abundance and accuracy of the term values data set still does not allow involving them into deperturbation routine. In present study we report observation of $c^3\Sigma^+ \to a^3\Sigma^+$ transitions in laser-induced fluorescence (LIF) applying $c^3\Sigma^+ \leftarrow X^1\Sigma^+$ excitation of rovibronic levels of $c^3\Sigma^+$ state by Ti-Sapphire laser radiation and observation of LIF dispersed by a Fourier-transform spectrometer with $0.03cm^{-1}$ resolution. An example of the observed LIF spectrum is given in Fig., left panel. The right panel represents the extended data field containing present new data (empty red circles) and data from [3] (black points). As is seen, the present data are extending the range of energy E' and of rotational quantum numbers N'. We will continue data acquisition in order to include them into a full scale deperturbation analysis together with $B^1\Pi$ and $b^3\Pi$ states (the b-B-c complex).

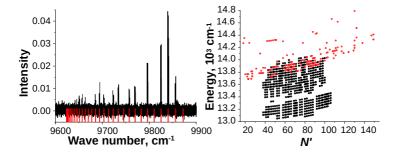


Figure 1: (left panel) - LIF transition $c3\Sigma+\to a3\Sigma+$ from level (N'=26, E'=13693.159 cm-1); (right panel) - $c3\Sigma+$ state term values as dependent on rotational quantum number N'; black points - from Ref. [3], red empty circles - present experiment.

We acknowledge support from the Latvian Council of Science Project No. lzp-2018/1-0020.

References

[1] T. Shimasaki et al, Phys. Rev. A. 98, 043423 (2018).

- [2] I. Birzniece et al, , J. Chem. Phys., 138, 154304 (2013).
- [3] J. Szczepkowski et al, JQSRT, 204, 131 (2017).

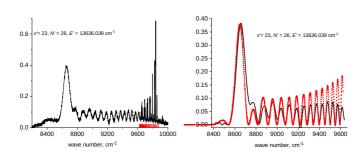
Analysis of oscillation structure in bound-free $c^3\Sigma^+$ - $a^3\Sigma^+$ transitions of KCs

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When the laser-induced fluorescence (LIF) transitions in diatomic molecules occur from the bound upper electronic state to the repulsive lower state part above the dissociation energy, the spectrum is changed from discrete to continuous. The respective bound-free part of LIF spectrum is modulated by oscillation structure as was first shown in [1] for $(2)^1\Pi \to a^3\Sigma^+$ LIF in NaK. Such spectra may supply the missing empirical data about the repulsive wall of the ground state potential [2], which implies the accuracy of dissociation energy determination, as well as the transport properties (viscosity, diffusion). In our studies we recorded and analyzed $c^3\Sigma^+ \to a^3\Sigma^+$ LIF spectra in KCs molecules excited by $c^3\Sigma^+ \leftarrow X^1\Sigma^+$ transition. An example of spectrum recorded by Fourier-transform spectrometer is presented in Fig., left panel. A comparison with the quantum mechanical simulation, which involves the empirical $c^3\Sigma^+$ potential from [3] is presented in Fig., right panel (solid line – experiment, dashed line - simulation). As is seen, though the positions of oscillations can be reproduced, the analysis has to be elaborated in order to describe the overall structure, for which we plan to determine a more accurate $c^3\Sigma^+$ potential accounting for interaction with $B^1\Pi$ and $b^3\Pi$ states.



University of Latvia team acknowledges support from the Latvian Council of Science Project No. lzp-2018/1-0020.

- [1] D. Eisel et al, J. Chem. Phys. 71(5), 2005 (1979)
- [2] M. Masters et al, J. Chem. Phys. 92 (10), 5801 (1990)
- [3] J. Szczepkowski et al, JQSRT (2017), 204, 131 (2017)

Intensity distribution in transitions from the A b complex to singlet and triplet ground states in RbCs

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We observed the $(A^1\Sigma^+ - b^3\Pi) \to a^3\Sigma^+$ transitions in laser-induced fluorescence (LIF) from the spin-orbit mixed A-b complex to the first triplet $a^3\Sigma^+$ state in the RbCs molecule. The transitions appeared to be extremely weak, being by about 3 orders of magnitude less intensive than the $(A^1\Sigma^+ - b^3\Pi) \to X^1\Sigma^+$ transitions to the singlet ground state. To our best knowledge these transitions have not been observed previously. The $(A^1\Sigma^+ - b^3\Pi) \to a^3\Sigma^+$ transitions were induced by Ti-Sapphire laser and recorded applying the highest possible detection sensitivity of IFT-125 Bruker Fourier-transform spectrometer, facilitated by an appropriate system of optical filters. Relative LIF intensity distribution (A-b) to a (see Fig., right panel) and (A-b) to X (see Fig., left panel) and a/X branching ratio was determined after calibration of detection system sensitivity within $8250-11700cm^{-1}$. The experiment was supported by ab initio full relativistic calculations. Both experimental and theoretical results can be useful to setup a laser assembling of RbCs molecules from ultracold Rb and Cs atoms applying stimulated Raman adiabatic passage (STIRAP) a to (A-b) to X scheme. University of Latvia team

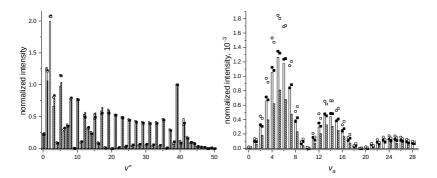


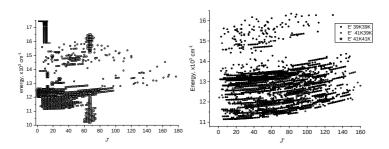
Figure 1: Intensity distributions in doublet P, R progressions of LIF progressions from the common A-b complex level J' = 97, E' = 11291.671 cm⁻¹ in 85RbCs: to $a3\Sigma + (right panel)$, to $X1\Sigma + (left panel)$. Points are ab initio calculations.

acknowledges support from the Latvian Council of Science Project No. lzp-2018/1-0020. References

The first excited states of K_2 revisited: first results

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The first excited $A^1\Sigma_u^+$ and $b^3\Pi_u$ states of the K_2 molecule that correspond to the 4S – 4P limit of separated atoms have been extensively studied by high-resolution spectroscopy methods. The existing data (see empty circles in Fig., left panel) have been summarized in [1] and processed by a 4x4 state deperturbation approach yielding the potential energy curves and spin-orbit interaction parameters. The data field used in [1] is fragmentary, no data existed for isotopes other than $^{39}K^{39}K$. New term values for low rotational quantum numbers J" near the dissociation limit (see black points in Fig., left panel) [2] have not been included in this fit. Our motivation to revisit the study was to considerably enlarge the abundance of data field by filling in the gaps in the interaction range of both states between 11 000 and 16 000 cm^{-1} and perform coupled-channels deperturbation, similar to the one used in [3] for Cs_2 , including all existing data. In the present study we excited $A^1\Sigma_u^+$, $b^3\Pi_u \leftarrow X^1\Sigma_q^+$ transitions in a potassium heat pipe and recorded laserinduced fluorescence (LIF) to the ground state. The spectra were recorded employing a Fourier-transform spectrometer IFT-125 Bruker with typical resolution $0.03cm^{-1}$. In addition, the data have been obtained by reanalyzing the LIF spectra previously recorded by us for KRb and KCs that contained a number of accidentally excited K_2 LIF. New data containing about 4000 term values obtained in present study are presented in Fig., right panel, among them about 500 term values belonging to ${}^{39}K^{41}K$ and about 20 to $^{41}K^{41}K$. The study is currently in progress.



We acknowledge support from the Latvian Council of Science Project No. lzp-2018/1-0020.

- [1] M. R. Manaa et al, J. Chem. Phys., 117, 11208 (2002)
- [2] St. Falke et al, J. Chem. Phys., 125, 224303 (2006)
- [3] A. Znotins et al, Phys. Rev. A. 100, 042507 (2019)

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Part III Optical materials and phenomena

Persistent luminescence of Mn2+ doped MgGeO3

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Persistent luminescence has wide range applications from science to practical life, luminophores are used in light sources, bioluminescent markers, electronics and so on. Persistent luminescence has been studied in the blue and green spectral regions, however much less research has been devoted to the red and infrared part of the spectrum, which is useable in medicine [1]. Recent publications [2], [3] has shown that MgGeO3:Mn $^{2+}$ is perspective material for red phoshorescence, however there has not been extensive studies about effect of Mn^{2+} concentration on properties and mechanism of persistent luminescence in this material.

In the course of this study ${\rm MgGeO_3:Mn^{2+}}$ samples with 10 different ${\rm Mn^{2+}}$ concentration were prepared by high temperature solid state reaction. The luminescent properties of ${\rm MgGeO_3:Mn^{2+}}$ samples were investigated by X-ray diffraction, thermally stimulated luminescence spectra, excitation and emission spectra, afterglow spectra etc. Material excited by X-rays or UV exhibit intense red luminescence with a peak around 680 nm. Most effective exhibit were measured with samples with ${\rm Mn^{2+}}$ concentration 0.5 mol % and 0.75 mol %, in 10mol % sample luminescence is still observable. Affter excitation by X-ray radiation samples continues to glow from 10 to 15 hours. Based on obtained results, conclusions about role of concentration of the ${\rm Mn^{2+}}$ has been drawn.

- [1] Y. Liu and B. Lei, "Persistent Luminescent Materials," in Phosphors, Up Conversion Nano Particles, Quantum Dots and Their Applications, Singapore: Springer Singapore, 2016, pp. 167–214.
- [2] Y. Katayama, T. Kayumi, J. Ueda, P. Dorenbos, B. Viana, and S. Tanabe, "The role of Ln 3+ (Ln = Eu, Yb) in persistent red luminescence in MgGeO3:Mn2+," J. Mater. Chem. C, vol. 5, no. 34, pp. 8893–8900, 2017.
- [3] Y. Katayama, T. Kayumi, J. Ueda, and S. Tanabe, "Enhanced persistent red luminescence in Mn2+-doped (Mg,Zn)GeO3 by electron trap and conduction band engineering," Opt. Mater. (Amst)., vol. 79, no. December 2017, pp. 147–151, May 2018.

Optical studies of diphenylsulfone and benzophenone derivatives as TADF compounds

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Organic light emitting diodes (OLED) are becoming more widely used in displays due to the high efficiency and lower production costs. TADF (Thermally activated delayed fluorescence) materials are the latest generation of OLED technology, which has 100The research work has been done for two types of TADF compounds considered - diphenyl-sulfone and benzophenone derivatives with carbazole groups. The aim of the study was to find potential blue light emitters. The presents of oxygen for such compounds is critical, because it interacts with the triplet states and significantly reduces the emission intensity. Therefore, to prove TADF properties of investigated compounds, the optical properties were examined in degassed and non – degassed solvents. Thin films were also prepared using spin coating method from the same solutions. For all compounds, the absorption and emission were measured in both solutions and thin films. The emission properties were different in the non-degassed and degassed solution, which proved the TADF properties of these compounds. The best photoluminescence quantum yield of 46 References

Doped AlN ceramics characterization by thermoluminescence technique

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Interaction of ionizing radiation or UV light with wide band materials results in ionization - transfer of the previously bound electrons and holes into conduction/valence bands and their trapping on the trap cetres. Supply of additional stimulation energy in the form of heat or light releases charge carriers, causing thermoluminescence (TL) or optically stimulated luminescence (OSL).[1] Aim of the given study is development of new prospective materials for dosimetry needs and elucidation of energy storage and recombination luminescence mechanisms in them. Dosimetric characteristics can be chosen based on thermal, spectral and timing properties of the TL and OSL of the measured ceramics, thus these methods were used for AlN ceramics with different concentrations of doped elements. The acquired results show a promising improvement of AlN ceramics properties by doping with yttrium because it shifts the TL curve peak to higher temperatures, thus decreasing the stored signal fading rate.

References

[1] Trinkler L. and Berzina B., A chapter in book Advances in Ceramics - Characterization, Raw Materials, Processing, Properties, Degradation and Healing. (pp. 59-82) Publisher: InTech, 2011.

[2] The present research has been sponsored from the Latvian Sciences Council Grant No. lzp-2018/1-0361.

Determination of Kerr effect origins by Z-scan polarization measurements

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For many years scientific groups have worked to move from an electro-optical telecommunication system to an all-optical one, with elements for optical data transmission, processing, and storage. Although independent elements for data transmission as well as processing have been presented, the all-optical system still lacks the necessary efficiency to compete with the electro-optical system. This is mainly due to third-order nonlinear optical (NLO) materials used in these systems not being efficient enough. In last year's organic materials have become very popular as they possess high third-order NLO effects and have high structure customization to fit for necessary applications. Due to this nonlinear optical material studies still is a very essential field.

In this work, we studied how polarization-dependent Z-scan measurements can be used to differentiate between various processes that induce refractive index changes. The main focus in this work was on picosecond and nanosecond laser measurements as they are the most common lasers used in literature. Due to the thermo-optical effect, the magnitude of the Kerr effect can be greatly overestimated if not correctly separated. At the same time, the Kerr effect has nuclear and electronic components that have different contributions in solution form and solid-state. To correctly predict organic molecules' applicability by studying it in the form of a solution, it is essential to separate both of these components. Acquired results were compared to quantum chemical calculations carried out with Gaussian 09 software to see how well calculations predict different components of the Kerr effect.

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Determination of light amplifying properties of red light emitting chromophores in thin films

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Red light emitting organic molecule 6- (tert-butyl) -4H-pyran-4-ylidenemalononitrile (DCM) can be used as a component in laser light amplifying medium [1]. The main issue of this molecule is its crystallization that reduces optical properties of the light amplifying system. Adding bulky groups helps to place the molecules further apart from each other.

In this work, thin films from 12 new synthesized DCM derivatives were prepared by spin coating method [2]. Absorption spectra, thickness, amplified spontaneous emission (ASE), photoluminescence quantum yields and compound stability were determined for each sample. Also, ASE measurements for samples with various film thickness were made. A nanosecond pulse laser and the variable stripe length method [2] was used to measure ASE.

Conclusions were made on the effect of electron acceptor and donor groups, and compound stability on ASE results. Results showed that the best compound is MWK-1TBQ with ASE excitation threshold energy value of 15 uJ/cm2 which is quite low compared with other threshold measurements done by other authors. For samples photoluminescence quantum yield values were in range from 2% to 18%. And comparison of the ASE results for samples with various film thickness is discussed.

- [1] M. Koschorreck, R. Gehlhaar, V. Lyssenko, M. Swoboda, M. Hoffmann, K. Leo, Applied Physics Letters Dynamics of a high-Q vertical-cavity organic laser, 87 (2005)
- [2] S.Forget, S.Chenais, Organic solid state lasers (Springer, 2013)

Optical and electroluminescence properties of Ir(ppy)3 molecular glasses in different hosts

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It is now considered that organic light emitting diodes (OLEDs) are the most appropriate technological solution for high quality displays [1]. One of the most investigated compounds applicable for wet processing is Ir(ppy)3 (tris(2-phenylpyridine)iridium) [2] due to its exceptional thermal and chemical stability and high photoluminescence quantum yield (Φ PL) of near 1.0. If it is vacuum deposited, Φ PL retains near a unity, in contrast, if it is solution-processed, aggregation of Ir(ppy)3 occurs, which leads to phase separation between the emitter and host material [3], as a consequence – efficiency of OLED decreases. To overcome this condition it has been determined that adding to Ir(ppy)3 bulky groups with purely isolating or charge transport functionality provides a physical barrier that suppresses the tendency of aggregate formation and helps to keep a large distance between emitter molecules. In this study Ir(ppy)3 and its structural analogues with a gradually increasing number of attached passive isolating groups were investigated. The molecular composition of these compounds consists of Ir(ppy)3 core and one (1TPY), two (2TPY) or three (3TPY) attached bulky triphenylmethane groups (TR). Absorption and emission spectra of all compounds did not show significant deviations among compounds, which means that adding TR groups does not greatly affect the electronic configuration of Ir(ppy)3 core. Onwards series of corresponding OLEDs with the solution-processed emissive layer containing electron deficient, hole deficient or balanced host material was created and analyzed. The best outcome in terms of turn-on voltage, current and power efficiencies and maximal brightness was achieved using balanced host material. Compounds investigated in this study can be used as emitters in solution-processable OLEDs, but further studies are required.

- [1] Chen, H.W., Lee, J.H., Lin, B.Y., Chen, S. and Wu, S.T., 2018. Liquid crystal display and organic light-emitting diode display: present status and future perspectives. Light: Science & Applications, 7(3), pp.17168-17168.
- [2] Baldo, M., Lamansky, S., Burrows, P., Thompson, M. and Forrest, S., 1999. Very high-efficiency green organic light-emitting devices based on electrophosphorescence. Applied Physics Letters, 75(1), pp.4-6.
- [3] Kim, Y.T., Seol, J.B., Kim, Y.H., Ahn, H.J. and Park, C.G., 2017. Correlation of Controllable Aggregation with Light-Emitting Property in Polymer Blend Optoelectronic Devices. small, 13(14), p.1602874.

Taking a Closer Look at Metal Halide Perovskites for High-Performance Solar Cells

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Over the past decade, the material class of metal-halide perovskites has been firmly established as the frontrunner for implementation in tandem structures with silicon, widely seen as the most realistic design for significantly boosting solar cell efficiencies and implementation in the near future. Perovskite/silicon dual junction cells have already been shown to reach efficiencies as high as 29.1%, surpassing the record efficiency of standalone silicon cells at 26.7%. A fundamental understanding of the in-operando charge carrier dynamics in these materials is, however, still lacking and a limitation towards the intelligent design of even higher performance optoelectronic devices. Back contacted designs for perovskite solar cells open up the possibility for detailed investigation of the photophysics of metal halide perovskites in full device structures, but have so far been scarcely explored. Here we propose a back contacted device design as a highly versatile platform for the study of charger carrier transport and recombination, as well as light-trapping strategies through a combination of optical and electrical characterization techniques. Using insights from this approach we hope to pave the way for pushing the efficiencies of perovskite-based solar cells towards their thermodynamic limits.

- [1] Pazos, L. M. et al., Science. 351, (2016)
- [2] Tainter, G. D. et al., Joule. 3, (2019)

Photoelectrochemical properties of ZnO/PDA nanostructures

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Polydopamine (PDA) is a novel biocompatible polymer with a number of functional groups. It can be used as layer for immobilization of biomolecules or reduction/oxidation reactions. ZnO is well known material with high room temperature photoluminescence, which can be used as optical sensor template. Forming of ZnO/PDA nanostructures can result in new photoinduced effects related to photoluminescence and photocurrent. Current work focuses on investigation and description of these effects. Optical and electronic properties of 1D ZnO/PDA nanocomposites are investigated by use of TEM, Raman, and FTIR spectroscopies, as well as photoelectrical measurements were done. Photoinduced effects have been observed and correlation between structural and optical properties of 1D ZnO/PDA nanostructures was performed. Electrochromic effect was observed as the optical properties-PL intensity- changed depending on the applied voltage. This methodology can be used for detection of biomolecules.

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- [1] Dong Yan et al, Polydopamine nanotubes: bio-inspired synthesis, formaldehyde sensing properties and thermodynamic investigation, J. Mater. Chem. A, 4, (2016) 3487-3493
- [2] Alla Tereshchenko, Mikhael Bechelany, Roman Viter, et al., Optical Biosensors Based on ZnO Nanostructures: Advantages and Perspectives. A Review, Sensors and Actuators B: Chemical, 229 (2016) 664-677
- [3] YanYang et al., Bifunctional polydopamine thin film coated zinc oxide nanorods for label-free photoelectrochemical immunoassay, Talanta, 166, (2017) 141-147
- [4] Jun Hee Kim et al, Polydopamine-assisted immobilization of hierarchical zinc oxide nanostructures on electrospun nanofibrous membrane for photocatalysis and antimicrobial activity, Journal of Colloid and Interface Science 513, (2018) 566-574

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Amblyopia and eccentric fixation

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Amblyopia or 'lazy eye' is impaired or dim vision without obvious defect or change in the eye. It is often associated with abnormal visual experience, most commonly strabismus, anisometropia or both, and form deprivation. The main task of amblyopia treatment is to ameliorate etiological factors to create a clear retinal image and, to ensure the participation of the amblyopic eye in the visual process. The treatment of amblyopia and eccentric fixation is usually associated with problems in the therapy [1]. Eccentric fixation is present in around 44 % of all patients with amblyopia and in 30 % of patients with strabismic amblyopia [2]. In Latvia, amblyopia is carefully treated in various clinics, but eccentricity diagnosis is relatively rare. Conflict which has developed relating to the relationship between the visual disorder and the degree of eccentric fixation in amblyopia should to be rethoughted, because it has an important bearing on the cause and treatment of amblyopia, and the role of the eccentric fixation in this case.

Visuoscopy is the most frequently used method for determination of eccentric fixation. With traditional visuoscopy, a fixation target is projected onto the patient retina, and the examiner asks to look straight directly at the center of the target. An optometrist then observes the point on the macula used for fixation. This objective test provides clinicians with direct observation of the fixation point of the eye. It requires patients to voluntarily fixate the target and assumes the foveal reflex accurately demarcates the center of the foveal pit. In the end, by having a very simple method to evaluate fixation, it is possible to indirectly evaluate treatment improvement, as eccentric fixation is always associated with reduced visual acuity [3].

So one may expect that if eccentric fixation in amlyopic eye is found with visuoscopy, then visual acuity should be less than 1.0 (in decimal units). With occlusion or another amblyopia therapy, one would expect both visual acuity and fixation to improve simultaneously, that is fixation would become more central. Consequently, improvement in fixation pattern by treatment is an indirect measurement of improvement of visual acuity. Evaluation of eccentric fixation in the child may be helpful in identifying amblyopia in children prior to measurement of visual acuity. This is very important because the earlier amblyopia is diagnosed – the better the chance of improving visual acuity.

- [1] Barrett B.T., Bradley A., McGraw P.V. (2004). Understanding the neural basis of amblyopia. Neuroscientist, 10:106-17.
- [2] von Noorden G.K. (1969). The etiology and pathogenesis of fixation anomalies in strabismus. Trans Am Ophthalmol Soc, 67:698-751.
- [3] Boyle J., Santamaria L. (2011). Two Case Studies: Eccentric Fixation and Amblyopia A Challenge to the Treating Practitioner. Aust Orthopt J, 43:24-28.

The effect of target shape on the quality of ocular fixation

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Even during fixation our eyes make small, involuntary movements. Physical properties of fixation targets can influence these small eye movements and the quality of eye-tracking data. For this reason, it is important to evaluate which target should be chosen as a calibration stimulus for the further creation of a calibration software for the multi-planar volumetric display.

Thaler et al. [1] studied various shapes of fixation target to evaluate what type of target minimizes involuntary eye movements during fixation. They evaluated seven different shapes to check whether the stability of fixation depended on this factor. Their results showed that the combination of circle and cross was the most appropriate shape of target for the stable fixation.

The aim of our study was to validate the results of Thaler et al. study using the same target shapes. Eye movements were recorded using the EyeLink 1000 Plus eye tracker. Fixation targets of four different shapes were chosen to be tested. Targets were presented in five distinct positions on the flat-panel display. Each stimulus was demonstrated for one second. Participants were asked to fixate their gaze on the stimulus. As a result, all tested stimuli ensured the similar fixation stability. Consequently, it was not possible to confirm conclusions reported in the earlier study.

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References

[1] Thaler, L., Schütz, A. C., Goodale, M. A., Gegenfurtner, K. R. (2013). What is the best fixation target? The effect of target shape on stability of fixational eye movements. Vision Research, 76, 31–42.

Volumetric image viewing strategies of medical professionals

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Nowadays, medical professionals examine a large amount of visual information in volumetric images, which consist of hundreds of image slices. The multi-slice image information is processed in a different way, compared to two-dimensional image viewing [1]. Two-dimensional images do not provide with all depth-related information making it difficult to judge the depth, shape and relative location of anatomical structures [2], however, volumetric images containing multiple slices facilitate image reading [3]. We were further interested to investigate what image viewing strategy medical professionals employ to review information presented in the three-dimensional way.

The research aim was to determine differences in volumetric image viewing strategies of medical professionals. 10 radiologists, 13 radiology residents and 24 medical students participated in this study. They performed non-medical visual search tasks with varying set sizes and target-distractor similarities on the multi-planar volumetric display (LightSpace Technologies, model: x1406). They could view the entire three-dimensional images or adjust the amount of image slices to be simultaneously shown on the volumetric display planes.

As a result, significant differences were observed in the volumetric image viewing strategy of experienced radiologists, compared to that of residents and students. The radiologists mostly preferred to view the entire three-dimensional image on the volumetric image. However, residents and students focused instead on a small amount of information and searched in a selective manner. In addition, the image viewing stategy of all participants was affected by the amount of information presented on the volumetric display. The revealed differences in image viewing strategy are important to be taken into account when designing the three-dimensional image navigation system for the new display which will be used for professional purposes.

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- [1] Van den Elsen, P. A., Pol, E.-J. D., Viergever, M. A. (1993). Medical image matching A review with classification. IEEE Engineering in Medicine and Biology Magazine, 12(1), 26-39.
- [2] Karatas, O., Toy, E. (2014). Three-dimensional imaging techniques: A literature review. European Journal of Dentistry, 8(1), 132.
- [3] Van der Gijp, A., Ravesloot, C. J., Jarodzka, H., van der Schaaf, M. F., van der Schaaf, I. C., van Schaik, J. P. J., ten Cate, T. J. (2016). How visual search relates to

visual diagnostic performance: a narrative systematic review of eye-tracking research in radiology. Advances in Health Sciences Education, 22(3), 765-787.

Accommodation response to stimuli of various contrast

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The 'steady-state' accommodation typically varies within a range of about plus or minus 0.5 D [1]. The range of these fluctuations should be lower than 0.5 D to study the dynamic accommodation responses when viewing multi-planar volumetric display [2] images. As far as the contrast of volumetric display images can be lower than that of flat-panel display images, we tested how the contrast of visual stimulus affected the short-term accommodation variation.

The purpose of this study was to measure the normal range of accommodation microfluctuations when the visual stimulus of two different contrasts was being viewed on a flat-panel display (Dell 24, model: P2419H) under binocular viewing conditions. We used the PowerRef3 plusoptiX R09 eccentric photorefractometer to record microfluctuations. Subjects viewed the visual stimulus at the distance of 45 cm. The Maltese cross (size: 0.9 deg) was used as a target on the dark background. It was presented at five different positions – in the center, and at the 5.2 deg field eccentricity in four directions (right, left, up and down). The luminance of Maltese cross varied resulting in the high and low contrast of the visual stimulus. The subjects were asked to fixate on the cross and follow it when its position on the screen was changed every ten seconds.

The obtained results indicated that the microfluctuations were larger for the high contrast stimulus, compared to the low contrast stimulus. However, this change in magnitude of the accommodation microfluctuations did not reach statistical significance. The further research should be done to assess the effect of measurement duration and visual adaptation on the accommodation response to stimuli of various contrast.

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- [1] Charman, W.N., Heron, G. (2015). Microfluctuations in accommodation: An update on their characteristics and possible role. Ophthalmic Physiol. Opt. 35, 476-499.
- [2] Osmanis, K., Valters, G., Zabels, R., Gertners, U., Osmanis, I., Kalnins, L., Kandere, U., Ozols, A. (2018). Advanced multiplanar volumetric 3D display. Proc. SPIE 10555, 1055510.

Computerized FM-100 colour test

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The incidence of congenital color vision deficiency in the female population amounts 0.5 %, while among men color vision deficits are detected in up to 8 % of cases. Studies have shown that chromatic sensitivity is changing during lifetime, i.e., chromatic sensitivity improves approximately till age 18, the 18 to 30-year age group shows highest chromatic sensitivity, after age 40 gradual decrease in chromatic sensitivity is observed (Paramei, 2012). Significant changes in color vision during life can be detected in people with eye diseases such as cataract (Ao et al., 2019), glaucoma (Niwa et al., 2014), diabetic retinopathy (Fong et al., 1999). Changes in color vision can be found after inhalation benzene and methyl alcohol vapors, and in patients who uses medicine like analgesics, antibiotics, neuroleptics, cardiac glycosides, antiarrhythmics and antihypertensives, as well as sleeping medications (Zrenner et al., 2007). Most of color vision tests, which are used in optometrician practices on daily bases aren't designed to monitor chromatic sensitivity changes, but to detect color vision deficiencies. The aim of this study is to assess whether FM-100 computerized color test could be used to determine type and severity of color vision deficiency, and to detect chromatic sensitivity differences among humans without color vision deficiencies. Our computerized FM-100 color test version does not require expensive color accurate monitors, thereby providing inexpensive and accurate tool for color vision screening and monitoring.

In scope of this research we have started to collect data to evaluate preretinal light absorption effects on color arrangement test results, i.e., effects of overall decrease of light intensity and spectrally selective light intensity decrease. During this study we will examine color vision of different age groups and clarify test scores for each of them. Study participant color vision were tested with computerized FM-100 color arrangement test version and as well with CCT (Cambridge Color test), anomaloscope, HRR and D15 color arrangement tests.

The study confirmed that computerized FM-100 color arrangement test version can be used to successfully evaluate type and severity of congenital color vision deficiencies. The results of computerized color arrangement test are in line with CCT, HRR, D15 and anomaloscope tests. FM-100 computerized test version can be used in optometrician practices on daily bases to assess and monitor color vision.

- [1] Zrenner, E., Hart, W. (2007). Drug-Induced and Toxic Disorders in Neuro-Ophthalmology.
- [2] Niwa, Y., Muraki, S., Naito, F., Minamikawa, Ohji, M. (2014). Evaluation of Acquired Color Vision Deficiency in Glaucoma Using the Rabin Cone Contrast Test. Investigative ophthalmology and visual science, Vol. 55, pp. 6686-6690.
- [3] Ao, M., Li, X., Qiu, W., Hou, Z., Su, J., Wang, W. (2019). The impact of age-related cataracts on colour perception, postoperative recovery and related spectra derived from test of hue perception. BMC ophthalmology, Vol. 19(N.1), pp:1-9.

- [4] Fong, D., Barton, F., Bresnick, G. (1999). Impaired color vision associated with diabetic retinopathy: Early Treatment Diabetic Retinopathy Study Report No. 15. Am J Ophthalmol., Vol. 128(N.5), pp:612-7.
- [5] G. Paramei (2012). Color discrimination across four life decades assessed by the Cambridge Colour Test. J. Opt. Soc. Am. A Vol. 29, pp: A290-A297

What additional information about near triad we can acknowledge if during clinical measurement of accommodation reserves the objective response is tracked?

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Most of the clinical tests that allow an optometrist to evaluate eye accommodation functions are either fully subjective or partially subjective therefore the result is achieved relying on patient's ability to discern changes in clarity or notice first blur. Previous research has highlighted potential other factors for example differences between push-up and push-down protocols or influence of depth of focus that altogether leads to the fact that subjective accommodation tests overestimate the true abilities of eye accommodation [1,2]. One of the most informative subjective clinical test is relative accommodation reserves, because it reflects not only maximum ability to stimulate or relax accommodation but also indirectly measure fusional vergence.

The aim of this study was for the first time qualitatively describe the pattern of accommodative response during binocular measurements of relative reserves and compare them with monocular measurements where vergence system is not involved. Twelve participants with emmetropia and mean age 26 ± 4 years participated in this study. For objective accommodation measurements we used an eccentric infrared photorefractor PowerRef~3 (Plusoptix GmbH, Nuremberg, Germany).

We have successfully demonstrated a method that allows in a laboratory setting to perform procedure closely similar to clinical measurement of accommodation reserves and record dynamic and objective accommodation response for each step until maximum ability to stimulate or relax accommodation is reached. Our results have demonstrated the use of additional information about microfluctuations and shown two cases where clinical measurement of negative relative accommodation is within normal values suggesting good abilities to relax accommodation, while objective response show pattern of excessive response. This method can be successfully used for specific research topics related to accommodation and vergence dysfunction.

- [1] Anderson, H. A., Hentz, G., Glasser, A., Stuebing, K. K., & Manny, R. E. (2008). Minus-lens-stimulated accommodative amplitude decreases sigmoidally with age: A study of objectively measured accommodative amplitudes from age 3. Investigative Ophthalmology and Visual Science, 49(7), 2919–2926
- [2] Wold, J. E., Hu, A., Chen, S., & Glasser, A. (2003). Subjective and objective measurement of human accommodative amplitude. Journal of Cataract and Refractive Surgery, 29(10), 1878–1888.

Reaction time measurement in perception of camouflage

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Camouflage is used by Military forces to make it difficult for opponents to notice and recognize them. It is important to find out, how efficient different camouflage models disguise under various environmental conditions, determining human attention and search ability [2].

When searching for an object subject mainly is focusing on area of interest.

Eye tracking devices are used to measure the gaze fixation and saccades of a people's eye by determining a person's conscious and unconscious part of attention. Analysis of eye movement parameters can tell us, whether camouflage effectively hide or attracts observer attention in a given environment. Eye movement researches are used to study human attention by performing various visual search tasks [4], but there are none of widely performed eye movement tasks with an eye movement device to determine camouflage efficiency [3].

The IviewX Red500 eye movement device was used to determine the efficiency of camouflage which is used by Latvian Army. It was found that eye movement analysis is an appropriate method for assessing the effectiveness of camouflage. First fixation time, average time spent looking at the camouflage element, and average fixation on camouflage element were different. It is possible to evaluate various parameters of visual attention and therefore evaluate the processes of visual perception in recognition of camouflage [1]. To measure camouflage effectiveness, it is still necessary to have measurements of other eye movement parameters (reaction time, saccadic movements, etc.), which will provide a more detailed analysis of the effectiveness of using camouflages. Therefore, the aim of this work is to evaluate the reaction time in camouflage visual search task in different environments at different seasons of the year by using eye movement system IviewX RED500 (SensoMotoric Instruments, Germany).

Four participants will take part in this study. Participants with visual acuity near 0.8 or higher and with good color vision will be selected for the study.

Four types of camouflage of the Latvian Army will be demonstrated on different natural environment backgrounds of an autumn. The location of the camouflage in the natural environment was 5m, 10m, 15m from the observer. Camouflage and natural environment images were taken with the camera Nikon D90 and stimulus were designed by using photo editing program Adobe PhotoShop. Participants will try to find some parts of camouflage on the photo of nature. When it will be noticed, participants will give signal by clicking computer mouse.

The camouflage recognition time are expected to vary based on the distance and the type of camouflage. When the camouflage is further from the observer, the participant's reaction time will be longer. Reaction time measurements with an eye movement system is an effective method of determining in which environment the camouflage is appropriate for.

Key words: camouflage, eye movements, reaction time

- [1] Agarelova, Z. Acu kustību analīze militārās kamuflāžas efektivitātes izpētē. Bachelor thesis (2019)
- [2] Hogervorst, M. A., Toet, A. & Jacobs, P. Design and evaluation of (urban) camouflage. Infrared Imaging Systems: Design, Analysis, Modeling and Testing. Proceedings of SPIE 7662 (2010)
- [3] Lin, C. J., Chang, C.-C. & Lee, Y.-H. Evaluting camouflage design using eye movement data. Applied Ergonomics 45(43), 714-723 (2014)
- [4] Muller, H. J. & Krummenacher, J. Visual search and selective attention. Visual Cognition 14(4-8), 389-410 (2006)

Assessment of user cognitive responses when viewing virtual 3D images and volumetric 3D images

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The development and further successful adoption of three-dimensional (3D) visualization technologies requires an accurate assessment of human factors. Recent studies mostly aimed to evaluate the impact of virtual 3D image viewing on user cognitive responses. We present the first comparative assessment of brain reaction when users are viewing different types of 3D images.

Virtual 3D images were generated on the conventional computer display (Dell, model: P2417H) using analyph technique. Volumetric 3D images were shown on the multiplanar display (LightSpace Technologies, model: x1405). The electroencephalography (EEG) was employed to evaluate brain physiological functioning and cognitive processing during relative depth perception of 3D images. Event-related potential (ERP) and frequency bands were analyzed. We used EEGLAB 2019.1.0. in conjunction with MAT-LAB R2015a for offline processing of eventrelated potential (ERP) and frequency bands.

As a result, there were several major differences revealed in user cognitive responses when viewing virtual 3D images and volumetric 3D images. The significantly higher activity of ERP was observed in the right parietal area (P4) for virtual 3D image viewing. Moreover, a considerably higher activity was revealed in the beta and gamma bands when users where performing relative depth judgement task with virtual 3D images. To sum up, the obtained results reflect that the greater cognitive effort is required to distinguish the relative depth of virtual 3D images, compared to volumetric 3D.

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- [1] Bang, J. W., Heo, H., Choi, J. S., & Park, K. R., ""Assessment of eye fatigue caused by 3D displays based on multimodal measurements," Sensors 14(9), 16467-16485 (2014).
- [2] Malik, A. S., Khairuddin, R. N. H. R., Amin, H. U., Smith, M. L., Kamel, N., Abdullah, J. M., Fawzy, S. M., Shim, S., ""EEG based evaluation of stereoscopic 3D displays for viewer discomfort," BioMed. Eng. Online 14(1), 1-21 (2015).