

## SLALOM 2022 Pitch session

	Name	Pitch title
1	<b>Kseniia Kosolapova</b>	Optical properties and energy structure of carbon dots based on citric acid and ethylenediamine depending on the type of polymer
2	<b>Milena Ramanovich</b>	Operator effective medium approximation for cylindrically symmetric layered structures
3	<b>Pavel Demakov</b>	Luminescent crystalline sponge: sensing properties, immobilization of flexible guests and substrate photochemistry within a porous host framework
4	<b>Pavel Alekseevskiy</b>	Metal-organic framework monolayer emission sources
5	<b>Anna Samsonova</b>	Crystal structure and vibrational properties of quasi-low-dimensional organic-inorganic lead halide perovskitoids
6	<b>Aleksandra Furasova</b>	Nanostructuring of n-i-p perovskite solar cells
7	<b>Danila Tatarinov</b>	Optical properties of Mn <sup>2+</sup> /Yb <sup>3+</sup> doped CsPbCl <sub>x</sub> Br <sub>3-x</sub> perovskite nanoplatelets
8	<b>Andrey Grachev</b>	Voltage-controlled topological states in magnonic crystal/PZT structure
9	<b>Aleksandra Boldyreva</b>	Steady state PL as an effective method to study radiation hardness of perovskite solar cells
10	<b>Marina Tepliakova</b>	Ultimate stability championship: rational design of double hole-transport layer enables high efficiency and stability of perovskite solar cells
11	<b>Semyon Bachinin</b>	Opto-electronic key based on film of HKUST-1

# SLALOM 2022

## PITCH SESSION PROGRAM

1

**KSENIIA KOSOLAPOVA** | ITMO UNIVERSITY

*OPTICAL PROPERTIES AND ENERGY STRUCTURE OF CARBON DOTS BASED ON CITRIC ACID AND ETHYLENEDIAMINE DEPENDING ON THE TYPE OF POLYMER*

The main aim of my research work is to identify the dependence of the influence of various functional groups on the carbon dots (CDs) surface on the charge and energy transfer. Polymers will act as additional substances: polyethylene glycol (PEG) and polyvinylpyrrolidone (PVP). Using the analysis of absorption and photoluminescence (PL) spectra, changes in highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels associated with changes in the geometric configuration of CDs during their transitions from the excited to the ground state will be considered. Models describing the features of the formation of the electronic structure and the surface of the CDs will be developed.

A comprehensive study of CDs with different surfaces will lead to obtaining information about the dependence of the size of the optical band gap on the morphology of CDs, which will further allow monitoring their electrical and optical properties.

2

**MILENA RAMANOVICH** | BELARUSIAN STATE UNIVERSITY

*OPERATOR EFFECTIVE MEDIUM APPROXIMATION FOR CYLINDRICALLY SYMMETRIC LAYERED STRUCTURES*

An operator approach to effective medium theory for homogenization of periodic multilayered structures was elaborated earlier. This approximation allows one to obtain effective material parameters of a homogeneous medium equivalent to multilayered one, in approximations of different order with respect to powers of ratio of the periodic cell thickness to the radiation wavelength. In this work, an operator approach to effective medium theory is generalized to cylindrically symmetric layered systems. To this end, solutions of Maxwell's equations in the form of the Born series expansions are used. Effective material parameters in the zeroth order Born approximation corresponding to an anisotropic dielectric are determined by equating the spatial evolution operators for the original structure and its effective alternative. It should be noted that for electromagnetic waves in cylinder's cross-section the effective material parameters differ from those in homogenized planar multilayered media. The results of our computations of the plane wave scattering by cylinders show that the obtained formulas describe an effective medium a little more precisely than formulas for planar multilayered media in the entire range of scattering angles.

**3**

**PAVEL DEMAKOV** | NIKOLAEV INSTITUTE OF INORGANIC CHEMISTRY, SB RAS

*LUMINESCENT CRYSTALLINE SPONGE: SENSING PROPERTIES, IMMOBILIZATION OF FLEXIBLE GUESTS AND SUBSTRATE PHOTOCHEMISTRY WITHIN A POROUS HOST FRAMEWORK*

A crystalline sponge method represents a convenient route for the single-crystal X-ray structural analysis of the molecules with a high degree of flexibility, which are hard to crystallize in a pure form. Encapsulation of such guests into a porous host with multiple intermolecular interactions allows to diminish molecular mobility of the adsorbed moieties, providing a necessary basis for their direct structure determination. Flexible metal-organic frameworks (MOFs) are recognized as valuable hosts for such method due to their high crystallinity possible to be retained even at a pronounced breathing, as well as high tunability of their chemical affinity and properties, unveiling further applications of the functional sponges in selective separations, sensing and data storage.

MOFs and metal-organic cages are perspective chemical nanoreactors due to pore size and shape limitations giving specificity and cleanliness of the encapsulated moiety transformation. In particular, such hosts have been successfully applied in diverse photochemical reactions allowed either to achieve unusual selectivities, when compared to the similar reaction in solutions, or to isolate and directly characterize unstable intermediates which are elusive without in-host immobilization. High guest-dependent adjustability of crystalline sponges unveils their advantages in such guest photochemistry.

This pitch discusses guest exchange in breathing MOF [Eu<sub>2</sub>(DMF)<sub>4</sub>(ttdc)<sub>3</sub>].4DMF (DMF = N,N-dimethylformamide, ttdc<sup>2-</sup> = thieno[3,2b]thiophene-2,5-dicarboxylate linker), which was obtained in our group, by means of structural and luminescent studies. Its characteristic Eu<sup>3+</sup>-related emission depends strongly on the nature of the included guest. In particular, a turn-off response was found upon inclusion of several aromatic aldehydes, while the structures of new adducts were unambiguously determined by single crystal XRD allowing to rationalize the guest impact of the host emission. UV-induced [2+2]-cycloaddition reactions for norbornadiene, 2-cyclopentenone and its derivatives encapsulated within a porous MOF sponge were performed with a successful direct SCXRD determination of the products, also revealing structure-driven selectivities.

**4**

**PAVEL ALEKSEEVSKIY** | ITMO UNIVERSITY

*METAL-ORGANIC FRAMEWORK MONOLAYER EMISSION SOURCES*

2D photoemissive materials have attracted high research interest due to their unique compatibility with an integrated planar photonic system, therefore, this type of materials ideally meets the requirements for planar photonic devices such as light-emitting devices, lasers, optical waveguides and emission sources for displays. Next to well-known inorganic 2D materials, 2D metal-organic frameworks (MOFs) stand out because of their high photoluminescence (PL) efficiency and tunable emission properties, based on structural design of the frameworks.

**5****ANNA SAMSONOVA** | SAINT PETERSBURG STATE UNIVERSITY***CRYSTAL STRUCTURE AND VIBRATIONAL PROPERTIES OF QUASI-LOW-DIMENSIONAL ORGANIC-INORGANIC LEAD HALIDE PEROVSKITOIDS***

Determination of the crystal structure of hybrid organic-inorganic halide perovskites is an important part of studying the electronic and optical properties of these materials. One of the most common methods for determining the crystal structure is X-ray diffraction analysis. However, it is not always available and is not applicable to all materials, which forces us to look for other methods. This is especially true for quasi-low-dimensional metal-halide materials manufactured by spin-coating in the form of thin films, as well as for materials whose X-ray diffraction analysis data are difficult to interpret for one reason or another.

It is possible to determine the local crystal structure of hybrid perovskites by measuring the vibrational properties of their organic cations, which do not have strong chemical bonds with the inorganic subsystem. In this work, we are trying to approach the solution of a global problem: establishing the influence of the crystal structure on the vibrational properties of organic cations. To solve it, we use relatively simple and sensitive experimental methods of vibrational spectroscopy, such as Raman and FT-IR spectroscopy, the data of which are confirmed by theoretical calculations using the density functional theory.

The materials under study were quasi-one-dimensional materials  $\text{PyPbI}_3$  and  $\text{PyPbBr}_3$ , where the pyridinium cation acts as an organic cation. The crystal structure of these perovskitoids is such that the nitrogen atoms in the pyridinium cations are not distinguishable by X-ray diffraction analysis. This is a result of the fact that in the crystal structure of these materials, nitrogen atoms are free to occupy not one specific position in the cation, but two. As a result, the infinite crystal structure consists of pyridinium cations with different positions of nitrogen - random or periodic, which the vibrational spectroscopy helps us to determine. We are also trying to investigate the influence of the inorganic subsystem on the pyridinium cation using vibrational spectroscopy.

**6****ALEKSANDRA FURASOVA** | ITMO UNIVERSITY***NANOSTRUCTURING OF N-I-P PEROVSKITE SOLAR CELLS***

Thin film perovskite solar cells (PSCs) present one of the most promising tools to get fast, cheap and environment friendly electricity sources for electricity generation in space, IoT applications or for household supply. Despite their rapid efficiency growth due to the careful selection of perovskite chemical composition and engineering of a cell design there are a number of unsolved problems with the charge generation and effective charge separation. This work summarizes our knowledge about PSCs mechanisms improvement by various semiconductor nanostructures: pristine and doped silicon nanoparticles, GaP nanowires. We studied n-i-p PSCs with various photoactive layers:  $\text{MAPbI}_3$ ,  $\text{CsFAMAPb}(\text{IBr})_3$  and  $\text{FAMAPb}(\text{ICl})_3$ .

**7****DANILO TATARINOV** | ITMO UNIVERSITY***OPTICAL PROPERTIES OF  $Mn^{2+}/Yb^{3+}$  DOPED  $CsPbCl_xBr_{3-x}$  PEROVSKITE NANOPATELETS***

Lead halide perovskite nanoplatelets (NPLs) have attracted significant interest in recent years because of their unique optical properties, such as a tunable position of emission wavelength, a narrow emission band, and a high photoluminescence quantum yield (PL QY). B-site cation doping is one of the most efficient approaches to precisely control the electronic and optical properties of perovskite NPLs. For instance, doping of perovskite nanostructures with  $Mn^{2+}$  and  $Yb^{3+}$  ions provides new PL bands at ~620 and 980 nm, respectively, which significantly expands their functionality. Doping with optically or/and magnetically active ions opens fundamentally new opportunities for the use of perovskite NPLs in photonic and optoelectronic applications, solar harvesting, and medicine. In the current study, we show that room-temperature post-synthetic doping may be efficiently applied for all-inorganic  $CsPbCl_xBr_{3-x}$  perovskite NPLs to achieve  $Yb^{3+-}$ ,  $Mn^{2+-}$ doped, and  $Mn^{2++}Yb^{3+}$  co-doped emitters. The morphology and chemical composition of the NPLs was investigated using electron microscopy and X-ray photoelectron spectroscopy. The optical properties of the obtained doped NPLs were thoroughly studied with steady-state and time-resolved spectroscopic techniques in both visible and near-infrared spectral ranges. It allowed us to obtain the main optical parameters of doped NPLs, including the position of characteristic spectral bands, PL decay times, and PL QYs in the visible and near-IR ranges. The proposed method of NPLs doping opens new opportunities for achieving perovskite nanostructures with tunable optical properties aiming their use in optoelectronics and photovoltaics.

**8****ANDREY GRACHEV** | SARATOV STATE UNIVERSITY***VOLTAGE-CONTROLLED TOPOLOGICAL STATES IN MAGNONIC CRYSTAL/PZT STRUCTURE***

We have experimentally studied the effect of electrical field control of the spin-wave spectra in magnonic crystal with piezoelectric layer. We revealed the mechanisms of controlling of spin waves by creating elastic strains localized in the region of maximums of the electric field strength. It is shown that when the absolute value and sign of the electric field are changed, it is possible to effectively control the properties of the propagating spin waves and the spatial distribution of the intensity of the dynamic magnetization in the multilayered structure. In result, the influence of the electric field materialize as the change of the magnonic gap size. We demonstrate that strong electric field can induce an accidental degeneracy and change of the topological phase transition. From an applied point of view, the results can be used to create a class of information processing devices, such as demultiplexing systems with spatial-frequency selectivity, controlled by an electric and magnetic field.



**ALEKSANDRA BOLDYREVA** | SKOLKOVO INSTITUTE  
OF SCIENCE AND TECHNOLOGY

*STEADY STATE PL AS AN EFFECTIVE METHOD TO STUDY  
RADIATION HARDNESS OF PEROVSKITE SOLAR CELLS*

Hybrid lead halides compounds is a group of materials that brings a new round of development for multijunction tandem solar cells.

Their outstanding opto-electronic properties make them attractive not only for terrestrial applications but also for the space industry. Space environment has much stronger radiation and consists of various high energy particles that can damage electronic equipment. It was recently shown that various perovskite materials are more stable under ionizing radiation than silicon. In this study, we continue exploring the radiation hardness of MAPbI<sub>3</sub> solar cells by means of steady state PL. We show that dependency of PL maximum intensity over radiation dose together with calculation of ideality factor gives a better understanding of recombination regime in the studied samples.



**MARINA TEPLIAKOVA** | SKOLKOVO INSTITUTE  
OF SCIENCE AND TECHNOLOGY

*ULTIMATE STABILITY CHAMPIONSHIP: RATIONAL DESIGN  
OF DOUBLE HOLE-TRANSPORT LAYER ENABLES HIGH  
EFFICIENCY AND STABILITY OF PEROVSKITE SOLAR CELLS*

Perovskite solar cells (PSCs) demonstrate impressive efficiencies of more than 25%, while reaching long-term operation stability remains a stumbling block for technology commercialization.

Application of double hole-transport layers (HTL) based on combination of organic and inorganic materials demonstrated its potential in boosting stability of PSCs. In this work the individual impact organic and inorganic components of double HTL is evaluated. In particular, four oxides in the highest oxidation states, namely MoO<sub>x</sub>, VO<sub>x</sub>, NbO<sub>x</sub>, and WO<sub>x</sub> in combination with polytriarylamine (PTAA) were investigated in PSCs with standard configuration. Using secondary ion mass spectrometry it was demonstrated, that the double layer prevents mitigation of volatile perovskite decomposition products from the structure, which is reflected in stable performance of photovoltaic devices.

At the second stage, a set of 46 conjugated polymers was investigated as organic component of double HTL. The benchmarking of materials in terms of their ability to enable stable performance allowed deriving requirements for polymeric HTL. Scanning electron microscopy of cross-sections of degraded devices revealed, that unstable devices undergo severe transformation of the bulk with formation of voids, which can be attributed to migration of volatile perovskite decomposition products due to poor encapsulation provided by HTL.

In sum, the performed studies shed a light on relationships between the structure and properties of hole-transport materials and the overall performance of PSC, allowing to propose a formula perfect double HTL for stable and efficient devices, which is a step towards the anticipated technology commercialization.



## *OPTO-ELECTRONIC KEY BASED ON FILM OF HKUST-1*

Optoelectronic components are today the most demanded area for industrial-oriented scientific projects. The high speeds of operation together with the ease of integration into traditional electrical circuits to increase the efficiency of the latter, opens up a huge potential for use. The traditional mechanisms of operation of optoelectronic components are usually associated with a change in the population of the energy levels of semiconductor systems, the manufacture of which often requires expensive and precision epitaxial technologies. An alternative mechanism that does not require the creation of complex semiconductor systems can be based on a reversible change in the ionic conductivity of some solid-state electrolytes, for example, metal-organic frameworks [1]. However, in the current works the times of change do not allow their use in computational optoelectronic circuits (on the order of 10 of minutes and higher [2]). We managed to obtain a reversible change in resistance from 2 MOhm to 10 MOhm in 5 seconds with a relaxation time of the order of 10 seconds. These times can be further reduced with further optimization of the structure design and reach milliseconds, based on the mechanism of such a switch (reversible breaking of coordination bonds with water molecules inside the pores), which was shown in the work [3].

References:

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