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2025

11th International Fall School on Organic Electronics

Book of Abstracts

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Moscow region, Russia
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11th INTERNATIONAL FALL SCHOOL ON ORGANIC ELECTRONICS – 2025 (IFSOE-2025)

Organizers

Division of Chemistry and Material Science of Russian Academy of Sciences

The Ministry of Science and Education of Russia

Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences (ISPM RAS)

Lomonosov Moscow State University (MSU)

MESOL LLC

Scientific program

1) ***Fundamentals of organic electronics:*** charge transport, modeling, photophysics, etc.

2) ***Design and synthesis of materials for organic electronics:*** organic conductors and semiconductors, dielectrics, substrates, etc.

3) ***Organic field-effect transistors:*** single crystal, polymer and monolayer OFETs, integrated circuits and related devices.

4) ***Organic light-emitting devices:*** OLEDs and OLETs, white light-emitting devices, TADF devices, organic lasers.

5) ***Organic and hybrid solar cells:*** small molecules and polymer photovoltaics, tandem cells, perovskites-based photovoltaics, etc.

6) ***Organic sensors:*** physical (pressure, temperature, photo, etc.) sensors, chemo- and biosensors.

7) ***Characterization techniques:*** various spectroscopy, microscopy, and x-ray scattering techniques, charge mobility measurements, thermal and surface analysis, HOMO and LUMO evaluation, biomedical applications, etc.

8) ***Technologies of organic electronics:*** printing of organic materials and devices, roll-to-roll techniques, ink formulations, encapsulation, etc.

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School program

The 11th International Fall School on Organic Electronics – 2025 Time Schedule

Moscow, Russia (GMT+3)

Time	Sunday September, 21	Monday September, 22	Tuesday September, 23	Wednesday September, 24	Thursday September, 25
8:00	**13:00** **Registration at ISPM RAS** **15:00** **Departure to Conference site** **17:00** **Hotel arrival Registration**	Breakfast			
9:00		**Sergey Ponomarenko**	**Dmitry Paraschuk**	**Maria Rosa Antognazza**	**Kostas Daoulas**
		Grigory Zyryanov	**Valentina Utochnikova**	**Raul David Rodriguez**	**Souren Grigorian**
10:00		**Ratheesh Vijayaraghavan**	**Alexander Romanov**	Oral talks 5	**Alessandro Troisi**
11:00		Coffee-break			**School Closing**
		Pavel Troshin	**Anna Koehler**	Oral talks 6	
12:00		**Maxim Kazantzev**	**Johannes Gierschner**	Sport activities	
		Oral talks 1	Oral talks 3		
13:00		**Lunch**			
14:00	**19:30** **School opening**	**Shinto Varghese**	**Artem Bakulin**	Excursion/Sport activities	14:00 Departure to Moscow
15:00		Oral talks 2	**Oleg Kharlanov**		
	19:45 **Vitaly Podzorov**		Oral talks 4		
16:00		Coffee-break + Poster session 1	Coffee-break + Poster session 2		
17:00	**20:30** **Welcome party**				
18:00		**Dinner**			
19:00		Sport activities		**Conference dinner**	

Sunday, September 21st

13:00 – 15:00	**Registration at ISPM RAS. Departure to conference site**
17:00 – 18:30	**Hotel arrival. Registration**
18:30 – 19:30	**Dinner**
19:30 – 19:45	**School opennig**
19:45 – 20:30	**T-1**. *Vitaly Podzorov.* Elucidating Intrinsic Electronic and Ionic Mobilities in Soft-Lattice Materials (Organic Semiconductors and Metal-Halide Perovskites)
20:30 – 23:00	**Welcome-party**

Monday, September 22nd

8:00 – 9:00	**Breakfast**
	Chair: *Pavel Troshin*
9:00 – 9:45	**T-2**. *Sergey Ponomarenko.* High Mobility Organic Semiconductors for Field-Effect Transistors
9:45 – 10:15	**I-1**. *Grigory Zyryanov.* Functional Polymers: (Mechano)Synthesis and Study of Photophysical and Applied Properties
10:15 – 10:45	**I-2**. *Ratheesh Vijayaraghavan.* Solid-State Aggregates of Ndis for Efficient n-Channel OFETs: Molecular Structure, Assembly and Function
10:45 – 11:00	**Coffee-break**
	Chair: *Grigory Zyryanov*
11:00 – 11:45	**T-3**. *Pavel Troshin.* Organic Batteries: Current Promises and Challenges
11:45 – 12:15	**I-3**. *Maxim Kazantsev.* Aryl-Containing Diazafluoren(On)Es for Organic Optoelectronics and Sensorics
	Oral talks 1.
12:15 – 12:30	**O-1**. *Daria Cheshkina.* Condensations of 4,5- and 1,8-Diazafluorenes
12:30 – 12:45	**O-2**. *Polina Shaposhnik.* New Siloxane Polymers with Grafted BTBT Groups as Materials for Organic Field-Effect Transistors
12:45 – 13:00	**O-3**. *Askold Trul.* Sensing Mechanism of Sensor Devices Based on Organic Field-Effect Transistors
13:00 – 14:00	**Lunch**
	Chair: *Maxim Kazantsev*

14:00 – 14:30	**I-4**. *Shinto Varghese.* Mechanical Conformity in π-Conjugated Molecular Crystals
	Oral talks 2.
14:30 – 14:45	**O-4**. *Valeriy Postnikov.* Polymorphism of Crystals Based on Linear Conjugated Molecules with a Central 2,1,3-Benzothiadiazole Fragment
14:45 – 15:00	**O-5**. *Irina Gudkova.* Synthesis and Phase Behavior Study of a New Organosilicon Tetramer with Octylhexyl-Substituted [1]Benzothieno[3,2-B][1]Benzothiophene Moieties
15:00 – 15:15	**O-6**. *Lev Levkov.* Conjugated Polymers Based on Alkylthiophene-Substituted Derivatives of Benzothieno[3,2-B][1]Benzothiophene
15:15 – 15:30	**O-7**. *Akim Shmalko.* Synthesis of C- and B-Anthracenyl-Ortho-Carboranes with Various Substituents in The Carborane Core
15:30 – 15:45	**O-8**. *Aleksander Mitroshin.* In Situ Synthesis of Solution-Processable TADF Polycarbazoles via Suzuki Polycondensation
15:45 – 17:15	**Coffee-break + Poster session 1 (*P-1 – P-17*)**
18:00 – 19:00	**Dinner**
19:00 – 21:00	**Sport activities**

Tuesday, September 23rd

8:00 – 9:00	**Breakfast**
	Chair: *Ratheesh Vijayaraghavan*
9:00 – 9:45	**T-4**. *Dmitry Paraschuk.* Multiresonant Luminophores for Light-Emitting Devices
9:45 – 10:15	**I-5**. *Valentina Utochnikova.* Lanthanide Based OLEDs
10:15 – 10:45	**I-6**. *Alexander Romanov.* Organometallic Complexes for Energy Efficient and Stable OLEDs
10:45 – 11:00	**Coffee-break**
	Chair: *Valentina Utochnikova*
11:00 – 11:45	**T-5**. *Anna Köhler.* Disorder, Aggregates and Vibrations in Spectroscopy
11:45 – 12:30	**T-6**. *Johannes Gierschner.* Bright or Dark - Regulation of Radiative vs. Nonradiative Processes in Novel Organic Materials
	Oral talks 3.
12:30 – 12:45	**O-9**. *Amira Nada Mechekkeme.* Weak Acceptor Approach Towards Blue TADF OLED-emitters Based on Carbazole Substituted Quinolines

12:45 – 13:00	**O-10**. *Olga Egorova.* Application of Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass-Spectroscopy in Research and Development of Organic Light Emitting Diodes
13:00 – 14:00	**Lunch**
	Chair: *Alexander Romanov*
14:00 – 14:45	**T-7**. *Artem Bakulin.* Monitoring Electronic Defects and Their Impact on the Device Performance of Processable Electronic Materials
14:45 – 15:15	**I-7**. *Oleg Kharlanov.* Electron-Phonon Interaction and Charge Transport in Organic Semiconductors
	Oral talks 4.
15:15 – 15:30	**O-11**. *Andrey Sosorev.* Novel Multi-Resonance Diindolophenazine Derivatives for Efficient Blue OLEDS
15:30 – 15:45	**O-12**. *Nikita Dubinets.* Multiscale Quantum Chemical Calculations of TADF-Luminophores in OLED
15:45 – 16:00	**O-13**. *Artem Toropin.* Comparative Analysis of The Applicability of Analytical Models of Charge Carrier Mobility in Disordered Organic Semiconductors
16:00 – 16:15	**O-14**. *Anna Saunina.* Effect of Exciton Transport and Dissociation Characteristics on The Performance of Photovoltaic Cell with Quantum Dot-Based Active Layer
16:15 – 16:30	**O-15**. *Yuriy Zhabanov.* Application of Theoretical and Experimental Structural Methods to Study Macrocycles for Organic Electronics
16:30 – 18:00	**Coffee-break + Poster session 1 (*P-18 – P-34*)**
18:00 – 19:00	**Dinner**
19:00 – 21:00	**Sport activities**

Wednesday, September 24th

8:00 – 9:00	**Breakfast**
	Chair: *Sergey Ponomarenko*
9:00 – 9:30	**I-8**. *Maria Rosa Antognazza.* Bio-Hybrid Photoactive Interfaces for Optoelectronic Modulation of Living Cell Fate
9:30 – 10:00	**I-9**. *Raul David Rodriguez.* Engineering 2D Material/Bio-Interfaces by Laser Forging
	Oral talks 5.
10:00 – 10:15	**O-16**. *Elena Poimanova.* Influence of Semiconductor Layer Thickness on The Operational Properties of Electrolyte-Gated Field-Effect Transistor
10:15 – 10:30	**O-17**. *Dmitry Godovsky.* Novel Non-Condensed Acceptors Based on 4H-Dithieno[3,2-B:2’,3’-D]Pyrrole and 4H-Cyclopenta[1,2-B:5,4-B’]Dithiophenen,S-Heterocycles with an Ethynylene Linker for Ternary Polymer Solar Cells with an Efficiency more than 15%

10:30 – 10:45	**O-18**. *Mukhamed Keshtov.* New 5,6-Bis(6-Fluoro-9H-Carbazol-3-Yl)Naphtho[2,1-B:3,4-B']Dithiophene Containing Π-Conjugated Wide Bandgap Donor Polymer Synthesized via Direct Arylation Polycondensation for Ternary Non-Fullerene Organic Solar Cells
10:45 – 11:00	**Coffee-break**
	Chair: *Dmitry Godovsky*
	Oral talks 6.
11:00 – 11:15	**O-19**. *Mikhail Uvarov.* Stable Radicals as Admixtures in The Active Layers of Organic Photovoltaic Cells
11:15 – 11:30	**O-20**. *Georgy Pakhomov.* Photoconductivity in thin films of oil porphyrins
11:30 – 11:45	**O-21**. *Polina Sukhorukova.* Design of Triphenylamine-Based Molecules with Anchor Group for Interfacial Layers of Perovskite Solar Cells
11:45 – 12:00	**O-22**. *Maria Sandzhieva.* Novel Organic and Hybrid Organic-Perovskite Composite Materials for Light Emitting Application
12:00 – 13:00	**Sport activities**
13:00 – 14:00	**Lunch**
14:00 – 18:30	**Trip to Abramtsevo Museum (optional) / Sport activities**
19:00 – 23:00	**Conference Dinner**

Thursday, September 25th

8:00 – 9:00	**Breakfast**
	Chair: *Dmitry Paraschuk*
9:00 – 9:45	**T-8**. *Kostas Daoulas.* Choosing The Right Formulation of Polymer-Based Inks for Printed Electronics: Opportunities and Challenges for Molecular Simulations
9:45 – 10:30	**T-9**. *Souren Grigorian.* Probing Thin Film and Nanostructure Morphologies with Surface-Sensitive X-ray Techniques
10:30 – 11:00	**I-10**. *Alessandro Troisi.* Modelling Charge Transport in Conjugated Polymers: The Challenges of High-Throughput Simulation and Mixed Ionic-Electronic Transport
11:00 – 12:00	**School closing**
12:00 – 13:00	**Sport activities**
13:00 – 14:00	**Lunch / Hotel check out**
14:00 – 14:15	**Departure to Moscow**

Poster session 1

Monday, September 22nd, 15:45

Aladeva, Aleksandra V.	P1	Features of Crystallization in Solutions of 4,7-Diphenyl-2,1,3-Benzothiadiazole and Its Derivatives with Terminal Alkyl Substituents
Bezsudnov, Igor V.	P2	A Two-stage Heating Mode for Thermomechanical Muscles Testing
Bobrova, Elizaveta A.	P3	New Triazine -Based Molecules for Organic Electronic Devices
Demianenko, Alena I.	P4	Anion Effect on Modulation of Synaptic Properties of Organic Biocompatible-Ionogel Electrolyte Neuromorphic Transistors for Deep Neural Networks
Dominskiy, Dmitry I.	P5	High-Vacuum Sublimation of Organic Semiconductor Materials for OLEDs
Filipenkov, Dmitry A.	P6	Impact of Organic Light Emitting Diodes Structure on The Charge Carrier Recombination Profile
Gaikov, Dmitry K.	P7	Creation And Research of Luminescent Compositions with Improved Characteristics for Light-Conversion Photoresists
Ghazaryan, Gagik S.	P8	Modeling The Behavior of Circular Dielectric Elastomer Actuators
Khitrov, Michael D.	P9	Theoretical Development of Diboraanthracene TADF Luminophores for Green OLEDs
Khmelnitskaia, Alina G.	P10	Development of Modified PDMS/MQ Composite as Dielectric Elastomers Actuators
Kleymyuk, Elena A.	P11	Synthesis and Study of The Properties of Host-Materials for the Emitting Layer of OLED
Koshelev, Daniil S.	P12	NIR OLED Based on Ytterbium Complexes with Schiff Bases
Krasnikov, Danila A.	P13	Baseline Drift Correction for OFET-Based Gas Sensors
Kuzmin, Ilya A.	P14	Influence of Intermolecular Interactions on The Electronic Absorption Spectra of SiF2-Etioporphyrin
Lavrinchenko, Igor A.	P15	Azolyl-Containing Luminescent Materials Based on Ortho-Carborane
Levitskaya, Alina I.	P16	Molecular Design of Polymer Materials Composed of Polyimide Matrix and Azochromophores Guests for Electrooptical Applications
Litvinenko, Daniil N.	P17	Geminate Pair Separation Probability in Organic Semiconductors: The Effect of Disorder and Energy Nonequilibrium (A Monte Carlo Study)

Poster session 2

Tuesday, September 23rd, 16:45

Mikhailov, Maxim S.	P18	New Diindolophenazine-Based Fluorophores with Highly Efficient Blue Electroluminescence
Nikerov, Dmitry V.	P19	New Method of Determining Charge Carrier Mobility in Thin Layers of Organic Crystals Using Time-of-Flight Technique
Poletavkina, Liya A.	P20	Synthesis, Study of Structure-Property Relationships and Comparative Analysis of New Annelated Push-Pull Semiconductors Based on Indolo[3,2-B]Indole and Benzothieno[3,2-B]Benzothiophene
Polyakov, Roman A.	P21	Optical Study of Non-Conjugated Polymers with Different Main Chain Nature for OLED Applications
Ponomareva, Anastasia V.	P22	Polymer Materials for Use in Light-Emitting Diodes
Popova, Vlada V.	P23	Terminal Groups Impact on The Properties of 2,1,3 Benzothiadiazole-Based Phenylene Derivatives
Potapov, Danil A	P24	Synthesis and Physicochemical Properties of Thiophene-Containing Derivatives of 4,5-Diazafluorene
Samburskiy, Denis E.	P25	Centrosymmetric Donor-Acceptor TADF-Emitters for Single-Layer OLED Exhibiting Aggregation-Induced Emission
Sorokina, Ekaterina A.	P26	Synthesis of Copolymers with Grafted Biotin-Containing BTBT Segments Based on Polysiloxane and Polystyrene
Stakanova, Daria E.	P27	Functional and Non-Functional Oligomers Based on 4,4’-Bis(2,1,3-Benzothiadiazole)
Starikova, Natalya D.	P28	Novel Chromophores, Incorporating 2,3-Diphenylthiophene Moieties
Tarakanovskaya, Daria D.	P39	Optoelectronic Property Prediction and Generation of Multi-Resonance Thermally Activated Delayed Fluorescence Molecules Using Graph and Multimodal Neural Networks
Titova, Yaroslava O.	P30	Semiconductor Properties of Novel [1]Benzothieno[3,2-b][1] Benzothiophene Derivatives in OFETs Prepared by Solution Processing
Trukhanov, Vasiliy A.	P31	Organic Light-Emitting Diodes Based on Thienyl-Containing Derivative of Tris(2,4,6-Trichlorophenyl)Methyl Radical
Zaborin, Evgeniy A.	P32	Grafted Polymers with Benzothieno[3,2-B]Benzothiophene (BTBT) Moieties as Side Groups: Prospects for High-Performance Organic Semiconductors
Dyadishchev, Ivan V.	P33	Synthesis and Properties of Π-Conjugated Molecular Liquids with Trihexylsilyl Terminal Substituents
Kuleshov, Bogdan S.	P34	Electrolyte-Gated Organic Field-Effect Transistor as a Perspective Platform for Detecting Metals in Aqueous Solutions

Tutorial lectures

Elucidating Intrinsic Electronic and Ionic Mobilities in Soft-Lattice Materials (Organic Semiconductors and Metal-Halide Perovskites)

V. Podzorov[1*], *V. Bruevich*[1]

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A vast body of works on field-effect transistors (FETs) utilizing various novel semiconductors is reported in the literature. However, the major current issue in the field is widespread erroneous mobility reporting (on the reproducibility crisis in modern science see, e.g., Ref. [1]). Two clear factors have been identified as contributing to this crisis. First, the majority of studies are performed on highly disordered, solution-processed materials that frequently lead to devices not well-described by the Shockley FET model.[2,3] This creates a lot of room for data misinterpretation and exaggeration of devices' metrics. Second, we currently witness a growing avalanche of blatant cheating in FET research, which concerns all types of actively investigated materials, aimed at reporting record-high mobilities.

In this talk, we will go through some examples of proper and improper mobility extraction practices in FETs and remind you about the safe mobility extraction protocols based on the classic Shockley FET model (the only available and ubiquitously used model for mobility extraction from FETs).[4,5] Specifically, important aspects and assumptions used in the Shockley model will be considered, with examples of how poor devices or extreme biasing conditions can lead to data misinterpretation and errors.[2,3,6]

In addition, substantial research effort must be dedicated by the community to elucidating the *intrinsic* charge carrier mobility of emergent electronic materials. This fundamental parameter is the ultimate (and, thus, the highest achievable) mobility for a given material, unaffected by static disorder, chemical impurities, or device imperfections. It is important for our understanding of a material's potential and true performance limitations. The intrinsic mobility can only be investigated by using high-quality FETs based on ultra-pure *single crystals* of the corresponding semiconductors (see, e.g.,[7,8,9]). Such studies are necessary, in particular, for mobility benchmarking and as a sanity check while evaluating results obtained in disordered thin-film transistors.

If time allows, we will also discuss some of our recent results on novel methods and device architectures for evaluating *ionic* mobility/diffusivity in metal-halide perovskites - the novel soft-lattice materials, where not only electronic, but also ionic motion is important for defining the behavior of devices.

This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0025401, as well as the Donald H. Jacobs Chair in Applied Physics at Rutgers University.

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High Mobility Organic Semiconductors for Field-Effect Transistors

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Organic secmiconductors are key functional materials for creating varoius types of field-effect transistors – organic field-effect transistors (OFETs), electrolyte gated organic field-effect transistors (EGOFETs) or organic light emitting transistors (OLETs). Their main property – field effect mobility – depends critically on the chemical structure, frontier energy levels, phase behaviour, crystal packing and processing techniques applied for preparation of the devices. In particular, good solubility and film forming properties are very important for solution processing of organic semiconductors. This can be achieved by rational design of solubilizing chains, including linear or branched alkyl, alkoxy-, alkyithio- and other substituents on particular positions of conjugated aromatic or heteroaromatic cores responsible for the semiconductor properties.

Recent advances in organic chemistry allows synthesizing a great variety of organic compounds possessing semiconductor properties[1]. The highest field-effect mobility amoung them show annulated molecules or those containing both annulated and linearly conjugated fragments. The latter class of organic semiconductors combine high mobility and bright luminescence in the bulk that is very promising for their application as active layers in OLETs. Tuning the energy levels of frontier molecular orbitals and bandgap in organic semiconductors via terminal substitution allows switching from the p-type to ambipolar and to the n-type OFETs[2,3].

This tutorial lecture considers classification and particular examples of high mobility organic semiconductors, peculiatities of their molecular design and chemical structures, physico-chemical properties as well as application in vatious types of field effect transistors – OFETs, EGOFETs and OLETs. Both literature examples[4-6] and organic semiconductors synthesized in ISPM RAS will be discussed[7-9]. Special attention will be devoted to the correctness of field-effect mobility values extraction and reporting taking into account various types of nonlinearities in OFET transfer characteristics according to Podzorov et al.[10] Peculiarities of the active layer formation for EGOFETs and their stability will be also highlighted [11,12].

This work was supported by Ministry of Science and Higher Education of the Russian Federation (contract No. D24-0493 within the framework of grant No. 075-15-2024-560).

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Organic Batteries: Current Promises and Challenges

E.V. Shchurik[1], *A.V. Mumyatov*[1], *Yu.I. Baluda*[1], *O.A. Krayevaya*[1], *P. A. Troshin*[2,1*]
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Using organic redox-active polymers as electrode materials for metal-ion batteries opens up principally new opportunities for the future development of the electrochemical energy storage technologies. First, organic materials are usually based on light elements (C, H, N, O, S) and, therefore, can enable much higher specific capacities compared to the salts and oxides of heavy transition metals. Second, organic materials are usually non-toxic and environment friendly, which makes easy their recycling as a common household waste. Third, polymeric materials are soft and, therefore, can operate at high charge and discharge rates thus leading to design of ultrafast batteries, which is challenging using crystalline inorganic cathodes and anodes. Moreover, mechanical properties of polymeric cathodes and anodes enable their application in truly bendable batteries for emerging generation of portable electronics. Finally, amorphous nature and simple redox mechanisms of polymeric electrode materials make them almost non-specific with respect to the type of mobile ions, while most of inorganic cathodes are constrained to only one specific ion matching the crystal lattice. This unique tolerance of organic electrode materials enabled successful demonstration of organic batteries operating with tens of different ions, in particular H^+, Li^+, Na^+, K^+, NH_4^+, Mg^{2+}, Ca^{2+}, Sr^{2+}, Zn^{2+}, Al^{3+}, etc. Thus, using organic materials, in particular, redox-active polymers, paves a way to the development of multiple new types of batteries for a broad variety of applications.

In this talk, we will provide an overview of our recent results on the design of organic and metal-organic redox active polymers and their application as electrode materials in lithium, sodium and potassium batteries. In particular, we will present ultrafast potassium batteries (charging/discharging in less than a minute) delivering high specific capacities and energy densities of ~600-900 W h kg^{-1} for the best organic cathode components. The polymer-based devices also demonstrated good cyclability with no capacity decay after a few thousand of charge-discharge cycles.

The obtained results suggest that organic electrode materials, while being at the infancy of their development, start to show commercially interesting performances thus attracting continuously growing attention to the new generation of post-lithium metal-ion battery technologies.

This work was supported by Ministry of Science and Higher Education of Russian Federation within the projects FFSG-2024-0008 (124013000743-3) and FFSG-2022-0001 (122111700046-3).

Multiresonant Luminophores for Light-Emitting Devices

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Organic light emitting diodes (OLEDs) are one of the most promising types of light-emitting electronic devices because of their low operating voltage, fast response, high brightness, and capability of achieving mechanical flexibility and/or semitransparency on flexible and/or transparent substrates. In recent decades, OLEDs have served as the basis of rapidly developing modern LED display technologies, gradually replacing traditional LCD technology. Despite of great progress in the OLED technologies, a number of challenges should be addressed to fully realize the potential of organic light-emitting devices.

One of the key problem to be solved is to find an optimal OLED luminophore that should provide ideally 100% quantum efficiency of electroluminescence (EL), long lifetime and high color purity, i.e. the narrow emission bandwidth. This combination of properties has not been realized in commercial OLEDs, e.g. phosphorescent luminophores can potentially reach 100% EL quantum efficiency but have relatively broad emission bandwidth (typically >40 nm ate half maximum). Since 2012, novel donor-acceptor fluorophores based on thermally assisted delayed fluorescence (TADF) actively have been studied in OLEDs. However, donor-acceptor TADF emitters suffer from relatively broad emission bandwidth.

This tutorial is focused on the latest achievements in one of the most promising, dynamic and young areas in the field of OLEDs, launched in 2016 and based on the so-called multiresonance fluorophores.[1] Fluorophores of this type potentially have a 100% quantum yield of luminescence and a narrow band, comparable to that for semiconductor quantum dots (~20 nm). A brief overview of the generations of OLEDs, the principles of operation of multiresonance luminophores, the features of their structure and their photophysical and luminescent properties are reviewed.[2,3] The achievements and problems in the field of multiresonance luminophores are critically analyzed and approaches to their molecular design are discussed.

The work was supported by Russian Science Foundation (project №24-49-02038).

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Disorder, Aggregates and Vibrations in Spectroscopy

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Photogenerated charges in films comprising the non-fullerene acceptor Y6 has sparked renewed interest in the underlying photophysical processes.[1,2] I shall discuss how to identify different chromophores in the absorption spectrum using Franck-Condon fitting. This will be applied to understand how different morphologies in a blend cause different solar cell efficiencies.[1,2] We shall also apply this to femtosecond absorption spectra to unravel the underlying processes.

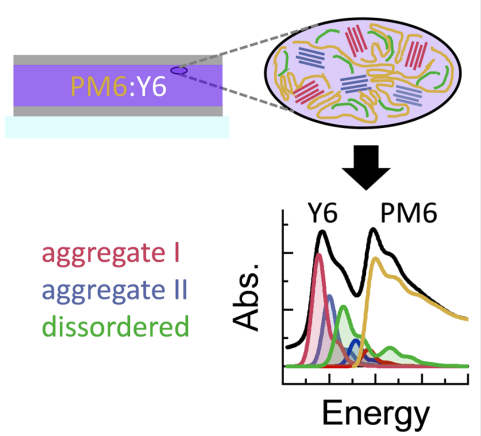

Fig. 1. Schematic showing a solar cell made with a blend of PM6 and Y6. The absorption spectrum is shown below. Indicated are in yellow the absorption from PM6, and in red, blue and green that from Y6 when it is aggregated in two different ways and when it is amorphous. These phases coexist in the blend with Y6

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Bright or Dark - Regulation of Radiative vs. Nonradiative Processes in Novel Organic Materials

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Conjugated organic chromophores have found immense interest in current materials research, and rapid progress has been seen over the past years, in particular due to advanced synthetic techniques. In any case, the quest for sustainable research demands pre-synthesis tailor-made targeted design beyond experimental (and computational) trial-and-error strategies. This can only be achieved by a thorough understanding of the underlying photophysical process combined with spectroscopic and computational techniques.[1]

A central figure of merit in the application of organic compounds is the fluorescence quantum yield Φ_F of the compounds, which is decided by the competition of radiative vs. nonradiative processes. This is not only key for obvious applications like OLEDs, OLETs, lasing, sensing, or bio-imaging, but also e.g. for photovoltaics.

For molecules in solution, nonradiative decay is mainly driven by internal conversion (IC; and subsequent vibrational relaxation; VR); this is frequently tackled via a 'Fermi's Golden Rule' (FGR) approach.[1] However, in the last years, it has become increasingly evident that FGR breaks down both in a quantitative as well as in a qualitative manner, in particular for systems with very effective IC. This was especially shown for compound families which establish an 'inverted energy gap law', sharply contrasting the prediction of FGR.[2,3,4] Instead, this has to be treated via conical intersections (CIs), which provides an accurate description of IC.

In molecular solids, in many cases, IC becomes a minor pathway, as the access to the CI often involves large amplitude motions which are effectively blocked in rigid environments;[2] this gives subsequently rise to 'Solid State Luminescence Enhancement' (SLE).[1] On the other hand, examples of active CIs in solid state samples have been identified, due to the absence of large amplitude motions on the path to the CI,[4] so that fluorescence quenching persists in molecular solids.

Nevertheless, the most crucial quenching pathway in molecular solids is trapping (at surfaces/interfaces), which becomes notorious in polycrystalline samples, while single crystals of the same materials are commonly highly luminescent.[1] The central role of trapping is largely underestimated in the community, and strategies how to achieve highly luminescent polycrystalline samples are thus addressed in the course of theseminar.

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[1] J. Gierschner et al. *Adv. Opt. Mater.* 2021, **9**, 2002251.

[2] (a) J. Shi et al, *J. Phys. Chem. C* 2017, **121**, 23166; (b) J. Shi et al, *Org. Chem. Front.* 2019, **6**, 1948; (c) M. A. Izquierdo et al, *Phys. Chem. Chem. Phys.* 2019, **21**, 22429.

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Monitoring Electronic Defects and Their Impact on the Device Performance of Processable Electronic Materials

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Organic and hybrid semiconductors, including organic–inorganic lead-halide perovskites, now underpin record-breaking single-junction solar-cell efficiencies (>26%) as well as highly tuneable light-emitting diodes (LEDs). Yet both perovskite and purely organic technologies continue to suffer from performance losses caused by trap-mediated recombination and field-dependent carrier imbalances. Crucially, these loss pathways emerge only under true operating conditions, where built-in and applied electric fields, charge-transport layers, space-charge accumulation, and ion migration (in the case of perovskites) reshape the local potential landscape in ways that differ strongly from neat films.

In this talk, I will outline our progress toward producing operando, molecular-scale "movies" of the electronic dynamics that govern both perovskite and organic devices. I will begin by showing how nanosecond transient-absorption spectroscopy allows us to track the real-time behaviour of free charge carriers; by analysing subtle features in the resulting spectra, we can map the internal electric field and pinpoint where carriers become either trapped or accelerated within the device stack.

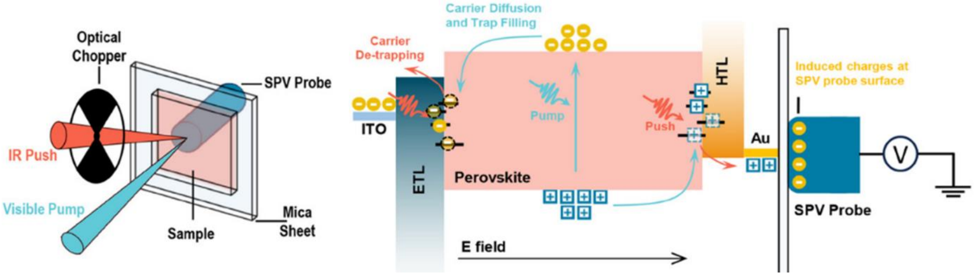

Fig. 1. IR optical control spectroscopy with photovoltage detection

I will then describe how these measurements are complemented by ultrafast mid-infrared pump–probe, or "optical-control," spectroscopy, which selectively excites and monitors bound excitonic and polaronic states—early-stage species that often lead to non-radiative losses in perovskite photovoltaic and light-emitting structures. Both action spectroscopy with photocurrent and photovoltage detection will be presented.[1,2]

Taken together, the two spectroscopic approaches provide a unified view of both free and bound charge populations under realistic operating conditions. Finally, I will show how coupling these experimental insights to drift-diffusion modelling closes the loop between microscopic dynamics and macroscopic performance, yielding concrete design rules for faster, more efficient optoelectronic devices.

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Choosing The Right Formulation of Polymer-Based Inks for Printed Electronics: Opportunities and Challenges for Molecular Simulations

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*e-mail: daoulas@uoi.gr

Unlike “conventional” printing, which focuses on pattern and color replication, printed films in organic electronics must retain the (opto-) electronic functionality intended by the chemical design of the deposited semiconducting polymer(s). The film functionality depends heavily on its structure, which results from a complex interplay between various phenomena that occur during delivery, positioning of functional inks on the substrates, and their subsequent drying. Therefore, obtaining devices with reasonable performance requires complex optimization[1] of numerous ink- and process-related parameters. Polymer-based inks are usually multicomponent mixtures, where the polymeric semiconductor is dissolved in a combination of solvents. Tuning the formulation of the ink, that is, the combination of the solvents that are mixed with the polymer, is among the basic strategies for achieving desirable ink parameters, such as viscosity, surface tension, wetting behavior, and drying time.

In this presentation we will highlight significant opportunities for using molecular simulations to optimize ink formulations. Several questions will be discussed, including the implementation of molecular simulations to understand mechanisms of polymer solvation. For example, such mechanisms may correlate with non-trivial dependencies of viscosity on the ratio of different solvents in the ink, see Fig. 1.

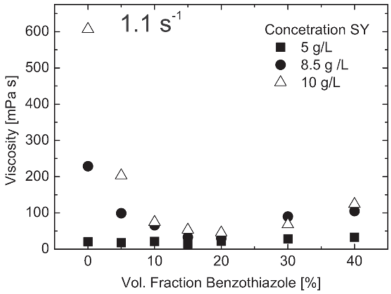

Fig. 1: Experimental data on the viscosity of a mixture of a PPV-based polymer (colloquially known as “Super Yellow”) with toluene and benzothiazole. The viscosity changes non-monotonously with benzothiazole concentration, especially at higher concentrations of polymer (SY). The figure is reproduced from ref[2].

At the same time, there are challenges. For example, the choice of the force-field may influence the predictions regarding solvation behavior. The investigation of dynamical properties with application-relevant molecular weights requires coarse-grained models. These simplified models, despite the reduction of molecular details, must be carefully designed to retain features that are essential for describing the structure of the solution and dynamics. Such challenges will be also discussed in the presentation.

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Probing Thin Film and Nanostructure Morphologies with Surface-Sensitive X-ray Techniques

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*e-mail: grigorian@physik.uni-siegen.de

Over the past few decades, surface-sensitive X-ray techniques have evolved into indispensable tools for the structural characterization of thin films and patterned nanostructures. Their non-destructive nature, combined with high spatial and temporal resolution, makes them especially valuable for probing complex systems at the nanoscale. Among these techniques, the combination of Grazing Incidence Wide-Angle X-ray Scattering (GIWAXS) and Grazing Incidence Small-Angle X-ray Scattering (GISAXS) has proven particularly powerful. Together, they provide complementary insights into the microstructural arrangement, molecular orientation, and interparticle correlations within various material systems.

This presentation will begin with a comprehensive overview of surface-sensitive X-ray scattering methods, outlining their fundamental principles and experimental geometries. A range of application examples will be presented, illustrating how these techniques can be employed to study structural properties in diverse classes of organic materials and blends.

The talk will also showcase recent experimental results obtained at advanced synchrotron radiation facilities, including time-resolved in situ studies that reveal dynamic structural evolution under external stimuli such as temperature, applied strain or electric field[1]. Finally, the discussion will address emerging opportunities enabled by novel nanofocused X-ray beamlines[2], which open new frontiers for high-resolution, real-time investigations of microstructure in organic and hybrid materials.

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Invited lectures

Functional Polymers: (Mechano)Synthesis and Study of Photophysical and Applied Properties

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[2]Postovskii Institute of Organic Synthesis UB RAS
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Functional polymers are applied in many fields, such as molecular sensorics and electronics, drug delivery systems, theranostics *etc*. In addition to the common approaches mechanochemically induced methods for the preparation of polymers are of high demand. Mechanochemical synthesis provides some advantages such as low or no solvent consumption, the accessibility of novel structures, and, most importantly, the avoidance of problems posed by low monomer/oligomer solubility and fast precipitation during polymerization.

In this report the most updated results on functional polymers synthesis will be presented, including mechanochemical approaches. Attention will be paid to the applications of the obtained materials as theranostics, sensory materials *etc*.

This work was supported by RSF (project № 25-73-30016).

I-2

Solid-State Aggregates of Ndis for Efficient *n*-Channel OFETs: Molecular Structure, Assembly and Function

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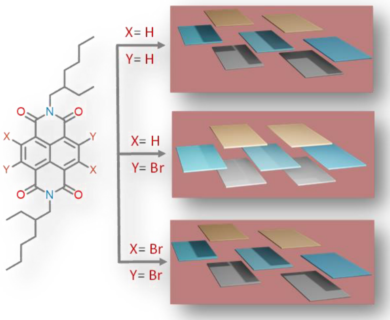
Economic and synthetically viable *n*-type organic semiconductor materials and solution-processed OFET devices with ambient stability and high electron mobility are rare. Converging all these desired requirements is still challenging; at the same, it is the need of the hour. Synthetic viability (less than three steps) and cost-effective starting materials are essential to achieve the same. Here, we discuss our strategy to achieve the right candidate with the above criteria. Napthalenedimiide (NDI) core structures were identified and we are revisiting the core-substitution strategy of the n-type planar aromatic core by easy synthetic route (two steps with 70% synthetic yield and 7 $/g material cost). The key highlights such as the solution-processed OFET devices with appealing electron mobility in the bulk film state (> 1 cm^{2}V^{-1}sec^{-1} with an on-off current ratio of 10^8) and ambient stability. A detailed investigation of the need for the unique supramolecular arrangement of the outperforming material in its Brickwork stack was systematically conducted and compared with two structurally similar model derivatives to assert our claims. Interlocked charge hoping units of the NDI core units in their Brickwork stack in the former case were found to be the principal reason for the superior device performance. Detailed electronic, spectroscopic and microscopic studies of the layers will be discussed.



This work was supported by DBT (project № BT/PR44972/NNT/28/1810/2021).

Aryl-Containing Diazafluoren(On)Es for Organic Optoelectronics and Sensorics

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Fluorene-containing materials are widely used in organic optoelectronics as bright emitters and excellent hole semiconductors[1]. For instance, spirobifluorenes were used in OLED as host materials for phosphors, as hole-transporting materials and as emitters; polyfluorenes are extensively used in OFETs and solar cells. Recently, diphenylfluorene was reported to have a good charge transport combined with the photoluminescence quantum yield up to 80% and excellent lasing characteristics[2]. However, diazafluorene-containing small molecules have been poorly explored though their nitrogen atoms could result in high electron affinity and electron transport[3,4]. Moreover, 4,5-diazafluorene-containing materials are promising for sensorics because of the N-coordination and protonation opportunities[3,5].

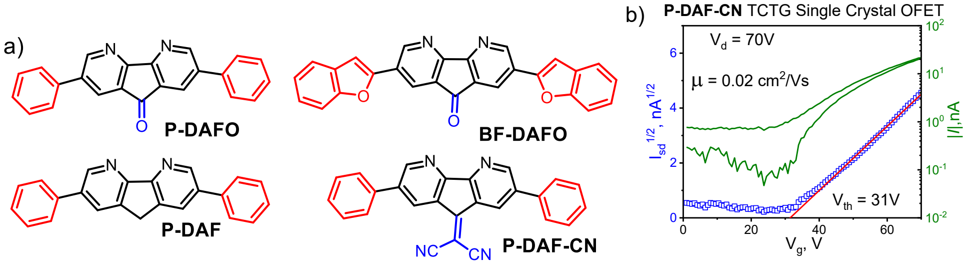

Fig. 1. a) structures of studied diazafluorene(on)es; b) transfer characteristics of P-DAF-CN single crystal OFET

Here, we report design, synthesis and detailed study of a series of 4,5-diazafluorene-derivatives containing different donor/acceptor groups and organic semiconductors based on these molecules. Crystal structures of all the materials were solved by X-ray diffraction revealing extensive π-stacking interactions. Further charge transport simulations indicated anisotropic charge transfer pathways. The materials were used as active layers in single-crystal and thin-film organic field-effect transistors (OFETs) demonstrating air-stable electron transport with charge carrier mobility up to 0.02 cm2/Vs for (2,7-diphenyl-4,5-diazafluorene-9-ylidene)malononitrile (P-DAF-CN). The good charge transport characteristics of this material stems from the lowest dipole moment among the molecules studied. Moreover, P-DAF-CN thin-film OFETs show a sensor response toward sub-ppm concentration of hydrogen sulfide. Therefore, 4,5-diazafluorene-based materials are promising organic semiconductors for air-stable n-channel OFETs and electronic nose applications.

This work was supported by RSF (project № 23-73-10015).

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Mechanical Conformity in π-Conjugated Molecular Crystals

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Flexible optoelectronics emerged as the need of the hour due to increasing demand for wearable and conformable devices. The key requirement of these devices is to withstand mechanical deformations without compromise in device performance. Crystalline organic π-conjugated molecules as active materials can offer an enhanced performance due to their superior charge and exciton transport properties over the semi-crystalline/amorphous counterparts. Organic molecular crystals are generally brittle and shattered into pieces on subject to subtle mechanical perturbation, which limit its application. A greater part of the fragile nature arises from the anisotropic packing of molecules in the crystal lattice, where the applied force dissipated in an asymmetric manner along the molecular planes resulted in the rapture. Seminal research work commenced by different groups brought about the consensus that the isotropic dissipation of applied stress is the key towards the mechanical compliance of the crystals. In a large variety of systems, the bending ability is due to a) interactions topology acting in the orthogonal directions b) corrugated structures and buffering weak and dispersive interactions and c) structural isotropy. However, most of the observations on mechanically compliant crystalline materials are serendipitous in nature. A more intense research is required to derive a rule of thumb design concepts to develop crystalline materials with mechanical compliances. Diverse structural motifs and synergetic interactions reported in the available literature that governs the mechanical compliances to applied stress in single crystals, untangling and differentiating the precise aspects responsible for mechanical conformity remains a major challenge. In my talk, I will be discussing our efforts in these directions develop mechanically compliant molecular crystals[1,2].

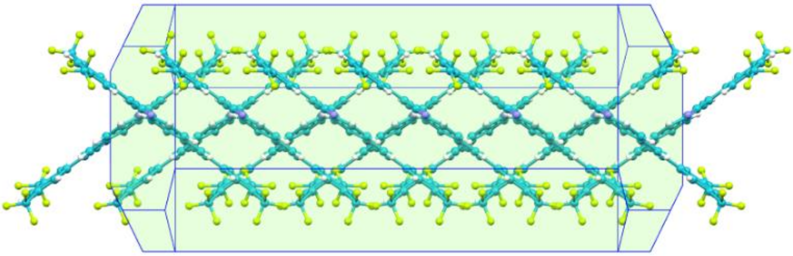

Fig. 1. Representative crystal packing that can sustain mechanical stress

This work was supported by SERB (project - CRG/2022/008007).

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I-5

Lanthanide Based OLEDs

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Organic light-emitting diodes (OLEDs) represent one of the most successful examples of molecular optoelectronics already translated into commercial products. Yet, for next-generation applications such as wearable and adaptive electronics, OLED technology still faces fundamental limitations. One of the most attractive but challenging directions is the use of lanthanide coordination compounds (LnCCs). They offer unique advantages – extremely sharp emission lines and access to the near-infrared (NIR) spectral region, where ytterbium-based complexes are particularly efficient. However, the practical use of LnCCs in OLEDs is hampered by their inherently long excited-state lifetimes, which restrict device efficiency and operational stability.

In our group, we have systematically analyzed the electroluminescence mechanisms of LnCCs and identified prolonged excited-state lifetimes as the key bottleneck limiting their performance. To address this issue, we explored different strategies to accelerate radiative deactivation pathways, with the most efficient solution being the introduction of plasmonic nanostructures. Incorporation of gold nanoparticles significantly enhanced terbium-based OLEDs, while anisotropic nanorods were shown to boost europium emission via strong localized surface plasmon resonance. These results demonstrate a clear pathway toward overcoming the long-lifetime barrier and unlocking the true potential of lanthanide-based emitters.

Taking advantage of these findings allowed us to develop color-tunable OLEDs (CTOLEDs**)**. By designing heterometallic coordination compounds, we realized dual-emissive devices in which europium (red) and ytterbium (NIR) emissions can be modulated in real time. The color output is dynamically tuned through intrinsic Joule heating, where Eu^{3+} emission undergoes progressive thermal quenching, while Yb^{3+} remains comparatively stable. This results in a luminescence intensity ratio (LIR) highly sensitive to temperature changes, enabling built-in optical thermometry with relative sensitivity up to 8% K^{-1} – one of the highest reported for molecular thermometers.

Electroluminescent studies at both cryogenic and ambient conditions confirm that the LIR–temperature dependence is robust and reproducible, whether triggered by self-heating under bias or external thermal stimuli. Importantly, spectral modulation is achieved without sacrificing device simplicity or stability, highlighting the practicality of this approach.

Thus, rational molecular and device design allowed to obtain highly efficient and multifunctional OLEDs, which provide a compact and energy-efficient platform for the next generation smart optoelectronic devices.

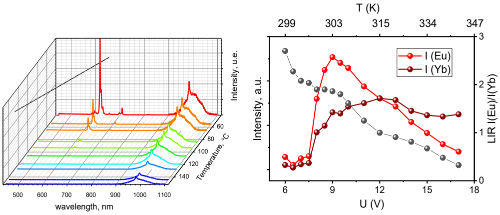

Fig. 1. a) Photoluminescence temperature dependence. c) LIR as a function of voltage and operating temperature under self-heating conditions

OLED manufacturing was supported by MSU Development Program

Organometallic Complexes for Energy Efficient and Stable OLEDs

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Two-coordinate coinage metal complexes with linear geometry L–Metal–X (L = carbene and X = anionic ligand, Metal = copper, silver or gold) have recently emerged as a new class of strongly photoemissive materials – Carbene Metal Amides (CMA).[1] We will discuss the advances in CMA molecular design to cover the full visible spectrum, UV-A (down to 380 nm) and near-IR regions (up to 850 nm). Advanced deep-blue Gold CMA emitters will be demonstrated to have radiative rates approaching 10^7 s^{-1}.[2] UV-A, deep-blue, red and near-IR CMA OLEDs with significantly improved device lifetimes (LT_{50} from several minutes to thousands of hours) will be presented to demonstrate the promising molecular design concepts and applied potential of the new CMA materials. New classes of the Carbene-Gold(I)-based emitters, such as Acetylides, Carboranyls and Aryls will be presented.[3,4,5,6] Comprehensive comparison across various classes of emitters will be based on the bond dissociation energies of the Metal–Ligand bonds to disclose the molecular designs leading to the best photophysical and OLED performance. New complexes will be demonstrated to show fluorescence, phosphorescence, TADF, two-photon triggered luminescence and energy transfer OLEDs.[3–6] We will discuss our very recent development of the advanced NON-host materials showing high stability, wide energy gap, and high triplet energy level over 3.3 eV.[7] NON-host materials unlock a true potential of the above mentioned gold-based luminophores by enabling highly energy-efficient OLED devices with EQE over 21% while producing a blue-shifted and narrow (60 nm) electroluminescence profile.

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Electron-Phonon Interaction and Charge Transport in Organic Semiconductors

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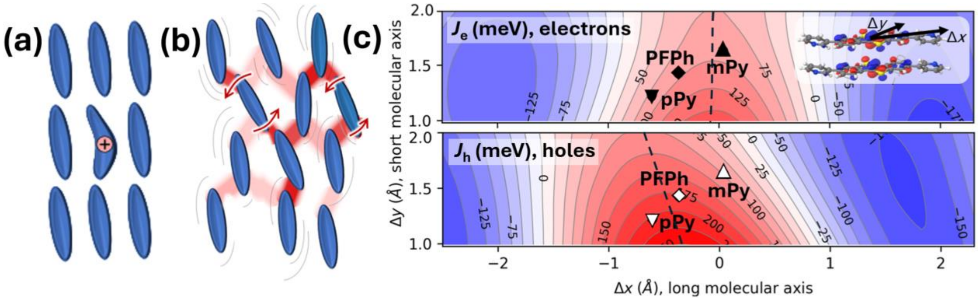

Fig. 1. Schematic representation of a small polaron (a) and a molecular crystal with dynamic disorder (b); transfer integrals in BTBT derivatives, R-BTBT-R, depending on the relative molecular positions (Δx, Δy) in face-to-face dimers, with dashed lines showing "sweet spots"

Organic semiconducting materials used in (opto)electronic devices allow for a vast variability via molecular design and the resulting changes in the crystal structure and/or morphology. With this versatility comes a challenge, since molecules as charge-transporting units exhibit a number of properties unusual for inorganic semiconductors, and these should be taken into account to design/predict a worthy organic material. Such properties and the corresponding transport mechanisms result from "softness" of organic molecules and crystals: a charge landing on a given molecule deforms it into a polaron (Fig. 1a), while periodicity of the lattice is constantly disturbed by thermal motion of its molecular sites (known as dynamic disorder, Fig. 1b). The two charge-transport aspects are manifestations of the strong electron-phonon interaction in organic materials[1,2]. In this talk, we give an overview of both aspects and further discuss strategies to minimize their detrimental impact on charge-carrier mobility, with the main focus on small-molecule organic crystals. Namely, we first dwell on the charge transport frameworks, such as the small polaron[i] and the transient localization scenario[3], elucidating their pros and cons from both the theoretical and computational points of view. Next, we discuss strategies developed in pursuit of suppressed electron-phonon interaction in organic crystals, having to do with the so-called "killer modes"[4] and "sweet spots" of crystal packing[5] (Fig. 1c). Another important strategy is associated with development of physics-inspired descriptors of weak electron-phonon interaction that could be used for screening of high-mobility semiconductors[6,7], in particular, those associated with the intermolecular interaction energy quantifying the "cohesive force" of an organic crystal[8]. Finally, we present a couple of such computational screening studies.

This work was supported by the Russian Science Foundation (project No. 22-72-10056).

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Bio-Hybrid Photoactive Interfaces for Optoelectronic Modulation of Living Cell Fate

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Use of light for selective and spatio-temporally resolved control of cell functions is emerging as a valuable alternative to electrical and chemical methods. Here, we propose the use of organic semiconductors as efficient and biocompatible opto-electronic transducers in the field of regenerative medicine. Devices able to selectively and precisely modulate the fate of living cells, from adhesion to proliferation, from differentiation to specific function, will be presented. Examples of practical applications include optical modulation of the activity of both excitable and non-excitable cells, the control of essential cellular switches like transient receptor potential and mechanosensitive channels, and effective modulation of calcium signaling for control of cell metabolism. Considered study-cases represent, to the best of our knowledge, first reports on use of organic semiconductors for optoelectronic modulation of the cell fate, with disruptive perspectives in regenerative medicine.

Engineering 2D Material/Bio-Interfaces by Laser Forging

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The integration of 2D materials into flexible materials is a cornerstone for wearable electronics. However, this material integration faces several challenges, including biocompatibility, scalability, and mechanical durability. The process begins with the exfoliation of 2D materials and proceeds through integration into the device to assess the performance of the final product. This presentation introduces the preparation of 2D materials, as well as a unique, single-step method to directly laser-process 2D materials for various purposes. Our approach harnesses precise laser-material interactions to simultaneously reduce and integrate precursors, such as graphene oxide[1,2], or chemically activate materials like MoS_2[3], thereby embedding them into the polymer matrix. The resulting structures exhibit exceptional adhesion and mechanical robustness, maintaining high electrical conductivity even after thousands of bending cycles, scratching, and chemical exposure. They also show enhanced photocatalytic performance. This maskless, direct-write method offers complete design freedom and is used to fabricate different high-performance (bio)electronic devices. We demonstrate ultrasensitive wearable sensors for monitoring breath and skin conductance, along with fully integrated, flexible electrochemical cells with laser-forged working, counter, and reference electrodes. Furthermore, the biocompatibility of the resulting materials enables their use as stable sensors on titanium implants and for direct on-skin monitoring of different bio-signals (ECG, EEG, EMG). We anticipate that this laser-forging platform will allow a scalable and cost-effective route to produce the next generation of durable, biocompatible, high-performance wearable and implantable bioelectronics with a wide range of 2D materials.

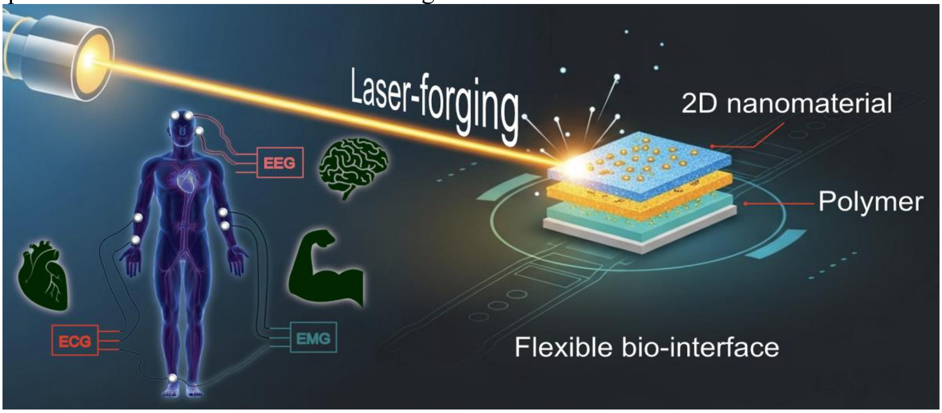

Fig. 1. Laser forging allows the free-form patterning of 2D nanomaterials into polymers for the creation of highly robust and biocompatible materials for wearable electronics.

This work was supported by the TPU Development Program Priority 2030.

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I-10

Modelling Charge Transport in Conjugated Polymers: The Challenges of High-Throughput Simulation and Mixed Ionic-Electronic Transport

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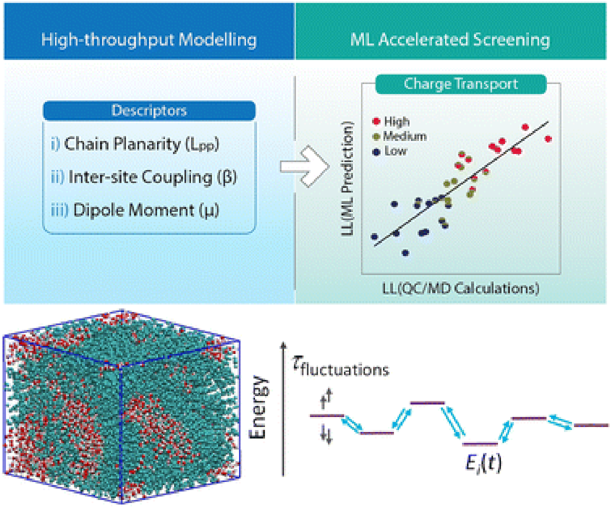
This talk will cover two related areas of modelling polymeric semiconductors for organic electronics. The first part will consider the deployment of classical modelling coupled with electronic structure[1] to study a large of set of semiconducting polymers with a homogenous methodology. Several technical innovations allow for the first time to design new polymers (rather than investigating them retrospectively). We reach a dataset size sufficiently large to enable the application of machine learning methods for the derivation of statistically meaningful structure-property relationships.[2] In the second part we consider the study of charge transport in organic polymeric materials with mixed ionic and electronic conduction (OMIEC) is proposed. The excess charge in doped polymers is very mobile and the dynamics of the polymer chain cannot be accurately described with a model including only fixed point charges. We introduced a new scheme based on the combination of MD and QM/MM to evaluate the classical dynamics of polymer, water and ions, while allowing the excess charge of the polymer chains to rearrange following the external electrostatic potential.[3] We find that the energy of the localized carrier states evolves in time: the trap states are short lived and energy barriers evolve over times. In other words ionic and nuclear dynamics is therefore driving the electronic dynamics rather than providing a static disordered landscape.[4]



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Oral talks

O-1

Condensations of 4,5- and 1,8-Diazafluorenes

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Diazafluoreneylidene derivatives attract a reasonable attention as functional materials for organic optoelectronics due to electron-withdrawing nature of nitrogen, planar structure, favorable for practical applications, and outstanding optical properties.[1] 4,5-Diazafluorene derivatives possess N-coordination ability, which enables applying in cation sensing, complexation,[2] security inks, and anti-counterfeiting applications.[3] Due to intramolecular non-covalent interactions, 1,8-diazafluorenylidene derivatives can form planar structures that exhibit solid-state luminescence enhancement.[4] The convenient method for synthesizing diazafluorenylidene derivatives is condensation of diazafluorenes with aromatic aldehydes or ketones. However, by now, only a few examples of these reactions involving 4,5- and 1,8-diazafluorenes have been reported.

In this work, the Knoevenagel condensation of 1,8- and 4,5-diazafluorenes with various aromatic aldehydes and ketones was studied under both basic and acidic catalytic conditions. The corresponding diazafluorenylidene derivatives were obtained in good yields. Only basic conditions (*t*-BuONa, DMF) were demonstrated to be applicable for reactions with acceptor-substituted aldehydes. Conversely, catalysis using ammonium acetate in acetic acid allowed us to obtain condensation products with both donor-substituted and acceptor-substituted aldehydes. These conditions gave higher yields than basic ones. Additionally, the first examples of the Knoevenagel reaction involving 1,8- and 4,5-diazafluorenes with aromatic ketones were synthesized and characterized.

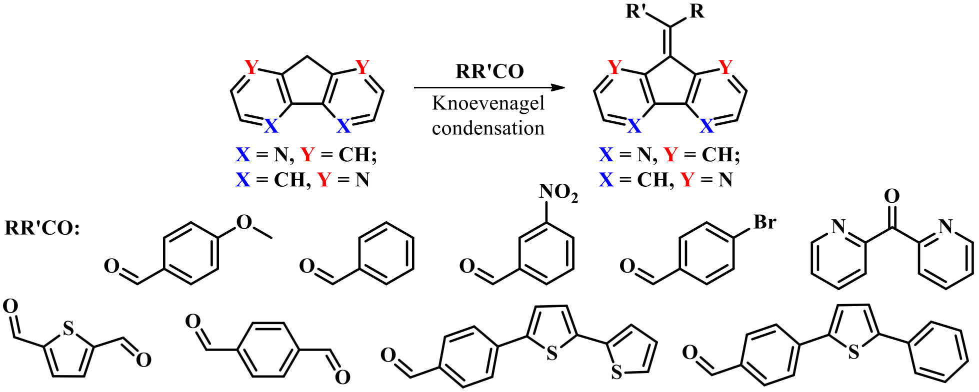

Fig. 1. General chemical structure of diazafluorenylidene derivatives

The conditions for Knoevenagel condensation were optimized to synthesize 1,8- and 4,5-diazafluorenylidene derivatives – promising materials for organic optoelectronics and sensing applications.

This work was supported by RSF (project № 23-73-10015).

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New Siloxane Polymers with Grafted BTBT Groups as Materials for Organic Field-Effect Transistors

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Organic semiconductor (OSC) materials can be divided into two main groups: small molecules and polymers. The first one allows to achieve higher charge carrier mobilities than polymer semiconductors, however, polymers have better processability and more stable thin film morphology than small molecule OSC. To combine the advantages of this two OSC types the blend approach is often used. However, in the most cases reported in literature to date, in blended OSC materials insulating polymers (such as polystyrene and PMMA) utilized as a polymer binders[1]. Due to vertical phase separation, such systems are ideally suited for top-gate organic field-effect transistors (OFETs)[2], but less convenient in case of printed contacts, which mostly used with bottom contact architecture. For such applications, semiconductor polymers capable of co-crystallizing with small molecules are of considerable interest.

In this work, the new siloxane polymers with different contents of grafted BTBT groups were synthesized and characterized. Such side groups have similar structure with widely used small-molecule OSC C8-BTBT and were designed to facilitate embedding of C8-BTBT into polymer matrix. Various polymer – C8-BTBT ratio were investigated to obtain the optimal material composition. It was demonstrated that using of the synthesized polymer allowed increasing the stability of OSC film morphology comparing to only C8-BTBT OFETs, which lost its field-effect properties after a month of storage in ambient conditions.

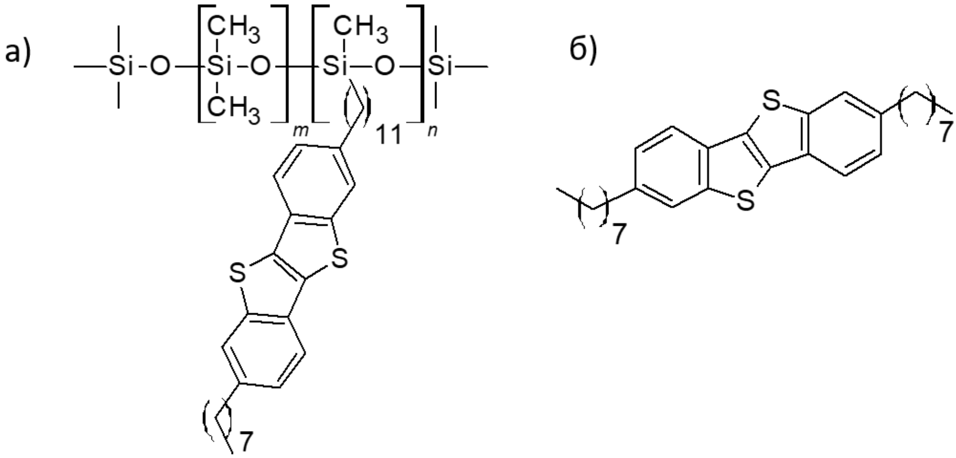

Fig. 1. a) Structure of new siloxane polymers; b) structure of C8-BTBT

This work was supported by RFBR (project № 19-73-30028).

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Sensing Mechanism of Sensor Devices Based on Organic Field-Effect Transistors

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S.Ch. Toirov[1], *M.S. Polinskaya*[1], *O.V. Borshchev*[1], *M.S. Skorotetcky*[1],
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Organic field-effect transistors (OFETs) are highly sensitive to the composition of the environment air due to the direct interaction between the thin semi-conducting layer of the OFET and the analyte[1] Despite a large number of works in this area, there is still no understanding of the general mechanism of operation of such sensor devices.[2,3] Most part of researches proposes that analyte molecules are sorbed on the semiconductor surface and caused the change of electrical characteristics of the OFET by interaction between semiconductor and analyte. However, there is currently no complete understanding of how exactly these interactions occur and what properties of the analyte or semiconducting molecules affect them. In this work, OFETs based on various benzothienobenzothiophene derivatives will be presented and discussed. The findings allowed to suggested that the sensitivity of the devices depends on the density of free charge traps, and the higher the density of free traps, the higher the sensitivity.[4] I addition, it was found that the sensitivity is mainly determined by the difference in the energy levels of the semiconductor and analyte, and the closer the levels, the higher the sensitivity.[5] At the same time, it is noted that the morphology and semiconducting molecules packing can also significantly affect the sensitivity of the OFET (in the case of sensitivity presence according to the proximity of energy levels).

These observations will be presented in detail in the talk, and further development of this topic will be presented to generalize these findings to a larger amount of devices.

This work was supported by the Russian Science Foundation (project No. 19-73-30028-P).

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Polymorphism of Crystals Based on Linear Conjugated Molecules with a Central 2,1,3-Benzothiadiazole Fragment

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U.S. Kirilina[3], *O.V. Borshchev*[2], *M.S. Skorotetsky*[2], *E.A. Svidchenko*[2], *N.M. Surin*[2]

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[2]Institute of Synthetic Polymer Materials RAS
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Linear conjugated molecules with a central 2,1,3-benzothiadiazole (BTD) fragment are of interest for optoelectronics and photonics as thermally and chemically stable highly efficient luminophores[1,2]. The molecular structure of these compounds is characterized by the absence of a center of symmetry and the presence of conformational flexibility, which causes the asymmetry of intermolecular interactions in the crystal and often leads to the presence of several unique structural units – conformers in the unit cell ($Z'>1$) and [1,2,3]. The indicated features of the molecular structure of linear 2,1,3-benzothiadiazole compounds significantly increase the probability of the formation of polymorphic modifications of the monotropic type with different optical-fluorescent characteristics (conformational polymorphism). Moreover, if in weakly nonequilibrium conditions one phase is usually formed, then in strongly nonequilibrium crystallization conditions the appearance of new polymorphic phases is often observed. On the one hand, the presence of phase instability in highly nonequilibrium conditions has a negative effect on the homogeneity and continuity of thin crystalline coatings. On the other hand, the presence of several structurally identified polymorphic phases provides a unique opportunity to thoroughly investigate the fundamental relationship between the conformational states of the molecule and the optical-fluorescent properties. Moreover, identifying the conditions for the preferential growth of a particular polymorphic modification opens up the possibility for various technical applications.

The report presents the results of a study of the growth, structure, thermal and optofluorescence properties of crystals based on linear 2,1,3-benzothiadiazole molecules. The tendency of compounds to polymorphism is analyzed in relation to the structure of the conjugated core of the molecule and the presence of certain terminal groups of substituents.

This work was supported by Russian Science Foundation (project № 22-13-00255-P), https://rscf.ru/en/project/22-13-00255/.

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O-5

Synthesis and Phase Behavior Study of a New Organosilicon Tetramer with Octylhexyl-Substituted [1]Benzothieno[3,2-B][1]Benzothiophene Moieties

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The development, synthesis and study of the properties of new organic semiconductor materials is a promising area of development in science. Such materials can be used as active layers for the creation of organic field-effect transistors (OFTs)[1], which in turn are used to create highly sensitive sensor devices[2].

One of the most promising low-molecular compounds, the derivatives of which are actively studied as organic semiconductors, is the [1]benzothieno[3,2-b][1]-benzothiophene (BTBT) molecule. Unlike polymer structures, BTBT oligoderivatives are characterized by a homogeneous molecular structure, which allows achieving the highest degree of their purity and, accordingly, leads to improved semiconductor properties.[3] It is known that the mobility of charge carriers in organic electronic materials increases with increasing conjugation length and crystallinity, but at the same time the solubility of such compounds is significantly reduced. The combination of alkyl-substituted BTBT derivatives with organosilicon groups increases the solubility of such semiconductor compounds and allows the creation of various linear, branched or dendritic architectures with interesting optical and electrical properties.[4,5]

In this research, tetrakis(3-(1,1,3,3-tetramethyl-3-(6-(7-octylbenzo[b]benzo[4,5]thieno[2,3-d]thiophen-2-yl)hexyl)disiloxaneyl)propyl)silane **D4-Hex-BTBT-Oct** (Scheme 1) was synthesized and characterized.

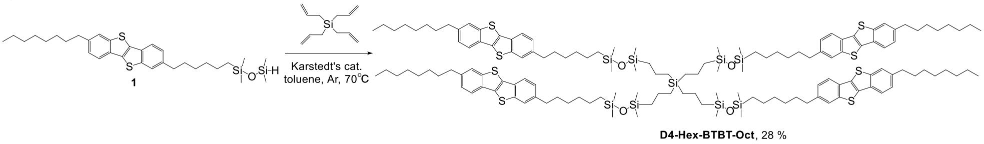

Fig. 1. Synthesis of the compound **3**

Synthesis of compound **1** was carried out according to literature methods.[6] The target compound **D4-Hex-BTBT-Oct** was obtained by hydrosilylation reaction in the presence of Karstedt catalyst. Study of thermal and thermo-oxidative stability of the obtained compound showed that it is stable in an inert medium up to 435°C, and in air up to 375°C. Study of phase behavior of the obtained compound **D4-Hex-BTBT-Oct** by DSC and POM methods reflects the presence of a reversible phase transition from the fan-shaped texture to the subsequent isotropization.

This work was supported by the Russian Science Foundation (project No. 19-73-30028).

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Conjugated Polymers Based on Alkylthiophene-Substituted Derivatives of Benzothieno[3,2-B][1]Benzothiophene

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Low-molecular semiconductors based on BTBT have been widely studied and high-performance optoelectronic devices have been created on their basis.[1] However, these are only laboratory prototypes typically produced using poorly scalable methods. A scalable technology for depositing functional layers via printing techniques is essential. The use of polymer semiconductors is particularly promising for this purpose due to the higher viscosity of their solutions compared to low-molecular-weight compounds. Compositions such as 2,7-dioctyl-BTBT-polystyrene have been extensively studied; however, their semiconductor properties degrade significantly over time due to phase segregation in the film[2]. A solution to this problem is incorporating BTBT fragments into the side chains or backbones of polymers.

The objectives of this work are the synthesis of conjugated polymers containing BTBT in the main chain and the evaluation of their potential application in organic field-effect transistors (OFETs). To achieve this, the following steps were carried out:

-Synthesis of BTBT derivatives with alkylthiophene groups, either unsubstituted at α-positions (1) or containing bromine atoms (2);

-Preparation of homopolymers from type 1 compounds via oxidative dehydrogenative polycondensation;

-Synthesis of copolymers with 2,5-thiophenediyl and 1,4-phenylene units from type 2 compounds using cross-coupling reactions;

-Investigation of the molecular weight characteristics, thermal properties, and optical behavior of the obtained polymers and copolymers.

Novel polymers possess relative number-average molecular weights (M_n) ≥ 20 kDa and polydispersity indices (Đ) ≤ 2.3. Incorporation of BTBT-fragments into the polymer backbones was confirmed by ^{1}H and ^{13}C NMR spectroscopy.

The synthesized polymers demonstrate good stability, exhibit narrower band gaps compared to their low-molecular-weight analogues[3] and retain crystallizability, indicating their strong potential for applications in organic field-effect transistor.

The study was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation, State contract FFSM-2024-0003.

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O-7

Synthesis of *C*- and *B*-Anthracenyl-*Ortho*-Carboranes with Various Substituents in The Carborane Core

A.V. Shmalko[1*], *S.A. Anufriev*[1], *I.B. Sivaev*[1], *V.I. Bregadze*[1]

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Icosahedral twelve-vertex carboranes $C_2B_{10}H_{12}$ are compounds consisting of two carbon atoms and ten boron atoms bonded to hydrogen atoms. Carborane-based compounds are of interest in both medicine and materials science. Recently, work has been actively carried out on the synthesis of carborane-containing luminophores[1]. Representatives of this class of compounds, C-anthracenyl-*ortho*-carboranes, are very promising due to their high efficiency of solid-state luminescence and ease of preparation[2,3]. In order to study the effect of substituents at the carborane core on the luminescent properties of compounds, we obtained a series of carborane derivatives with substituents that have different electronic properties. The resulting compounds were introduced into the reaction of Ni-catalyzed cross-coupling with 2-bromoanthracene, resulting in a series of *C*-anthracenyl derivatives of *ortho*-carborane[4]. We have also proposed a method for synthesizing *B*-anthracenyl-*ortho*-carboranes containing a polyaromatic fragment at the boron atoms in different positions of the carborane core[5], which are promising compounds for studying their optical properties.

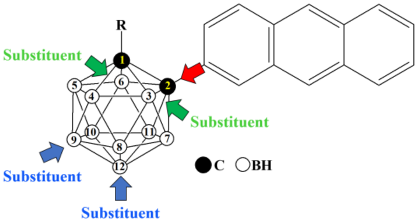

Fig. 1. Common view of anthracene-carborane dyad

The structure of the obtained compounds was confirmed by multinuclear NMR spectroscopy and mass-spectrometry. Single-crystal X-ray diffraction data were obtained for a number of derivatives.

This work was supported by RSF (project № 25-43-00072).

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In Situ Synthesis of Solution-Processable TADF Polycarbazoles via Suzuki Polycondensation

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Polycarbazole-based materials have emerged as an excellent platform for developing solution-processed OLED emitters with thermally activated delayed fluorescence (TADF), benefiting from their high-energy backbone triplet states. While conventional approaches require pre-synthesis of complex TADF luminophores before incorporation into the polymer matrix, we present a novel *in situ* strategy that directly constructs TADF-active polymers from simple, non-TADF monomers through Suzuki polycondensation. Our approach utilizes dibromo-triazine and diborolane-carbazole derivatives coupled with a 1,4-dioctyloxybenzene spacer to simultaneously achieve *in situ* formation of TADF-active tricarbazole-triazine (TCzTrz) moieties within the polymer backbone and enhanced solubility in toluene and chlorobenzene through octyloxy side chains.

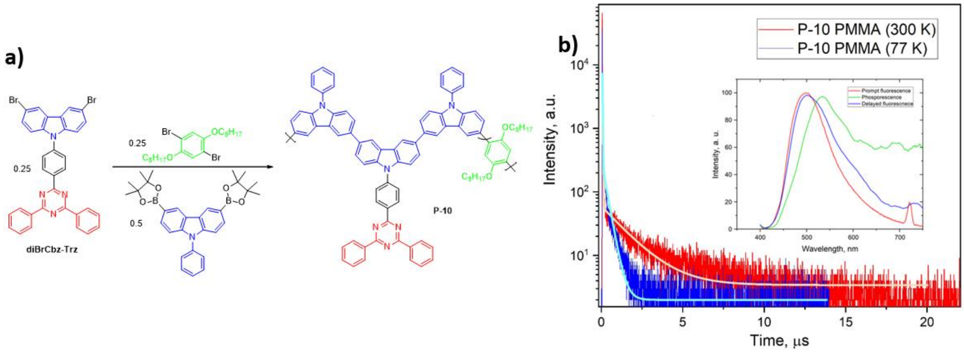

Fig. 1. a) Synthetic scheme of P-10; b) temperature dependences of transient PL of 10 wt% doped P-10 PMMA films. Insert – steady-state PL spectra (red), phosphorescence spectra (green), time-resolved PL spectra at room temperature (blue)

The resulting P-10 polymer demonstrates TADF property. Identity of photoluminescence (PL) and delayed fluorescence maxima ($\lambda_{PL} = \lambda_{DF} = 502$ nm) confirms emission from the same singlet state. Temperature-dependent lifetime studies shows decreased delayed component lifetime at 77K. Exceptionally low ΔE_{ST} of 0.03 eV enables efficient reverse intersystem crossing. Crucially, we demonstrate the essential role of aryl substitution at the carbazole nitrogen for achieving TADF properties. Control experiments with alkyl-substituted analogs showed complete absence of TADF characteristics, highlighting the necessity of phenyl group for proper electron density delocalization and low ΔE_{ST} formation.

This work was supported by Russian Science Foundation (project № 25-13-00300).

O-9

Weak Acceptor Approach Towards Blue TADF OLED-emitters Based on Carbazole Substituted Quinolines

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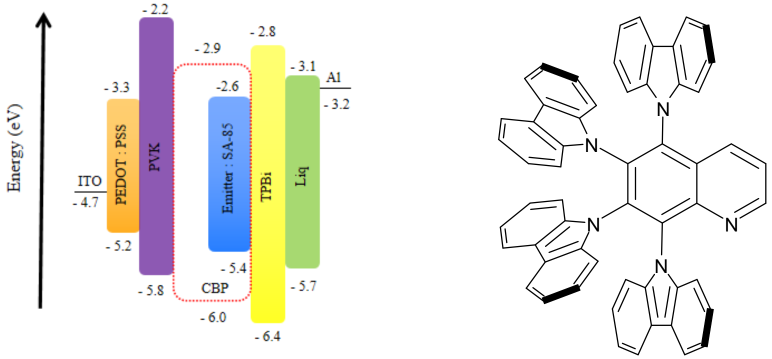
Organic Light Emitting Diodes (OLED) is an emerged light emitting technology, based on multilayered organic thin film structures. One of the key points contributing to OLED effectiveness is the optimization of the light-emitting layer to enable the harvesting of both singlet and triplet excitons. Thermally activated delayed fluorescence (TADF) is one of the promising approaches to improve triplets to singlet conversion via reverse intersystem crossing (RISC) and to increase OLED effectiveness.[1]

In this study, we introduce weak-acceptor molecular design strategy for solution-processed blue TADF emitters, based on carbazole substituted quinoline – **Cz4Quin**. For both non-doped and doped OLEDs were fabricated with the architecture ITO/PEDOT:PSS/ PVK/ emissive layer/ TPBi/ Liq/ Al and their optoelectronics properties were systematically characterized.



Cz4Quin

Fig. 1. Energy level diagram for OLED device and **Cz4Quin** emitter structure

The optimized device achieves a maximum external quantum efficiency (EQE) of 7% with sky-blue emission (peak wavelength $\lambda_{max} = 500$ nm, full-width at half-maximum FWHM = 76 nm) and a low turn-on voltage $V_{on} = 5.5$ V.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (no. FSUS 2021-0014) and by the Material science department of the Indian Institute of Science Bangalore India (IIsc).

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Application of Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass-Spectroscopy in Research and Development of Organic Light Emitting Diodes

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Organic light emitting diodes (OLEDs) have garnered enormous attention due to their undeniable advantages, such as high contrast ratio, wider viewing angle, better power efficiency and optimal thickness for flexible devices. However, a major technical challenge of OLED technology is limited lifetime of organic materials included into organic multi-stacking layer, often caused by partial thermal and chemical degradation during the manufacturing process. Degradation of emitting organic materials under high driving voltage applied to completed OLED device leads to pixel defects formation and reduce device's performance[1]. Additionally, excepting degradation of organic materials, mass-production (MP) of OLED small, medium and large-sized panels often have many different issues related to identification of unknown organic materials, polymers, particles and so on.

The common analytical methods for identification of individual organic materials and their mixture are often Nuclear Magnetic Resonance Spectroscopy (NMR), Liquid Chromatography combined with Mass-Spectrometry (LC-MS). However, these techniques have several limitations, such as sample quantity requirement, solubility in organic solvents and being time-consuming and costly.

Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass-Spectroscopy (MALDI-TOF) is well-established analytical techniques mainly used for biological propose like biopolymers identification. Nevertheless, MALDI-TOF is also a very fast and accurate method for identification of individual OLED compounds, entire OLED devices, polymers, pigments, quantum dots and particle contaminations present at various stages of OLED manufacturing.

Typically, MALDI-TOF spectrometers employ UV lasers (260-355 nm) for ionization. Most individual organic compounds used in OLED panels have a strong absorbance in UV-Vis region and do not require assisted matrix support for sufficient ion yield. Thus, the simplified Laser Desorption/Ionization technique (LDI-TOF) can be effectively applied for OLED material and panel analysis.

Another key advantage of LDI-TOF technique for OLED analytical propose is very simple sample preparation. Individual organic compounds can be spotted onto a sample target from organic solution, regardless of its quantity and solubility as LDI-TOF has an extremely low detection limit toward OLED compounds (nanogram scale). OLED panels can be analyzed directly without additional preparation, aside decapsulation (removing the protective layer).

Therefore, the LDI-TOF technique, adapted for OLED research and mass-production enables us to identify degradation products of individual OLED materials, examinate a chemical composition of OLED multi-stacking layer, polymers, pigments, quantum dots and various contaminations.

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Novel Multi-Resonance Diindolophenazine Derivatives for Efficient Blue OLEDS

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Organic light-emitting diodes (OLEDs) are the most successfully commercialized organic electronic devices. However, for blue OLEDs, there is still a tradeoff between efficiency, color purity and device lifetime. Recently, a novel class of emitters for such devices that can overcome these limitations, - multi-resonance fluorophores, - was suggested. Due to the rigid annulated conjugated core with embedded heteroatoms in certain positions, they show reduced electron-vibrational coupling resulting in narrow emission spectrum and hence pure color. Although several series of multi-resonance fluorophores were suggested, the structure-property relationships for these compounds are rather poorly studied, which hinders their rational design. In this study, we addressed theoretically and experimentally the impact of various substituents on the fluorescence properties of novel multi-resonance diindolophenazine (DIPz) derivatives. Specifically, we applied DFT modelling and revealed the most promising compounds of this series emitting in deep-blue range: PhDIPz (DIPz4), tBuPhDIPz (DIPz5), and MesDIPz (DIPz6). We then synthesized these compounds, studied their luminescent properties and tested the former in OLEDs as emitters (dopants) embedded in a popular anthracene-based host NaNaP-A. All the devices showed deep-blue emission (see Fig. 1 for color coordinates) with the maxima in the range 430-455 nm and pronounced vibrational structure, but were relatively narrow (55-62 nm). The characteristics of the DIPz-derivatives-based OLEDs were found to be comparable to those for the reference device based on a known multi-resonance fluorophore, pSFIAc1; one of the OLEDs based on the novel compounds, namely tBuPhDIPz, showed considerably higher EQE (Fig. 2), ~75% larger current efficiency and twice higher energy efficiency than the reference device. It was shown that addition of tertbutyl group to the phenyl substituents of PhDIPz negligibly affects the emission maximum, considerably reduces the spectrum width and significantly improves OLED characteristics, while three methyl substituents per phenyl ring result in blueshift of the emission spectrum and deterioration of OLED characteristics. We anticipate that the suggested fluorophores will serve as dopants for efficient deep-blue OLEDs, while the revealed impact of substituents on optical properties of DIPz derivatives will facilitate rational design of multi-resonance fluorophores.

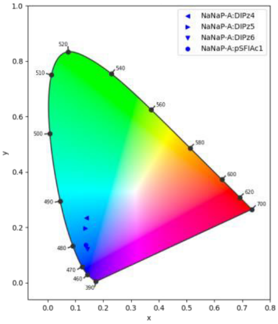

Fig. 1. CIE coordinates of the fabricated OLEDs.

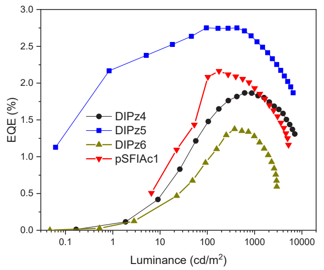

Fig. 2. EQE of the fabricated OLEDs as a function of luminance.

The study was supported by the Ministry of Science and Higher Education of the Russian Federation (project #FFSM-2025-0004).

O-12

Multiscale Quantum Chemical Calculations of TADF-Luminophores in OLED

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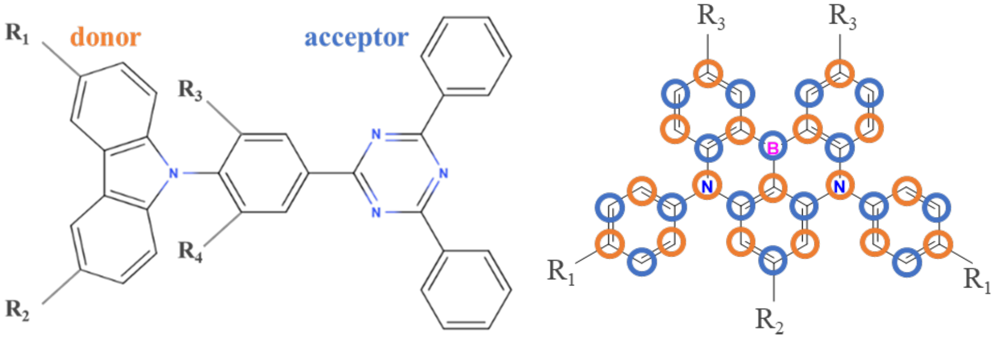
Organic light-emitting diodes (OLEDs) have seen transformative progress in recent years, driven in large part by the development of thermally activated delayed fluorescence (TADF) materials—commonly referred to as 3-rd generation emitters. Among the earliest and most extensively studied TADF systems are the donor–acceptor-type Cz-TRZ molecules and the multi-resonance (MR) emitters based on DABNA frameworks. Notably, the MR approach has emerged as the most effective strategy for achieving both narrow emission bandwidths and high photoluminescence quantum yields (PLQY), positioning it at the forefront of next-generation OLED emitter design.



(Cz-TRZ) **(DABNA)**

Fig. 1. Structures of studied TADF-luminophores and it’s derivatives

In this study, the influence of substituents on donor–acceptor-type Cz-TRZ-based and multi-resonance (MR) DABNA-based TADF luminophores, with explicit consideration of their local environments was investigated. Fluorescence spectra for both bulk dopants and dopant–host systems were calculated using time-dependent density functional theory (TD-DFT). All hybrid and doubly hybrid functionals examined yielded consistent trends in the $S_1 \rightarrow S_0$ transition energies. Accordingly, the computationally efficient B3LYP functional was selected for subsequent multiscale simulations. The structural stability of the luminophores was further evaluated using bond dissociation energy (BDE) analyses.

This work was supported by the Ministry of Science and Higher Education within the State assignment (project № FFSM–2025–0004).

Comparative Analysis of The Applicability of Analytical Models of Charge Carrier Mobility in Disordered Organic Semiconductors

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Transport of charge carriers is one of the basic physical processes underlying the functioning of organic electronics. The key characteristic of transport is mobility. The Monte Carlo (MC) method enjoys universal confidence, but generalization of MC results to the parameter range where the model used in the MC calculation is not applicable leads to errors. Analytical approaches, although they contain additional simplifying assumptions, facilitate the analysis of the dependence on numerous parameters. Most analytical results are based on different versions of the transport level concept and effective temperature, while percolation effects are taken into account in different ways[1,2,3]. A generalized multiple trapping and release model has recently been proposed that does not require explicit calculation of the transport level[4,5]. It allows the analysis of different energy distributions of hopping centers (not only a Gaussian distribution)[4] as well as not only quasi-equilibrium but also nonequilibrium transport[v]. It is instructive to test the results of this model by comparing them with reliable MC data over a wide range of disorder parameters using the popular Gaussian energy distribution of hopping centers as an example. In a recent paper[6], the MC simulation data taking into account off-diagonal disorder were fitted with a fairly simple analytical expression for the mobility as a function of temperature, field strength, and carrier concentration. In the present work, the previous analytical models[2-4] are modified, where necessary, to take into account the off-diagonal disorder. The temperature dependences of the mobility obtained within these models for different values of the localization parameter are compared with the expression obtained in the paper[vi]. The comparison shows good qualitative agreement between the results of the work[vi] and the works[iv,v], as well as previous works[1-3], in a fairly wide range of parameters (the width of the energy distribution of the hopping centers, the localization radius of the wave functions). The areas of the best quantitative applicability of each model are determined.

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Effect of Exciton Transport and Dissociation Characteristics on The Performance of Photovoltaic Cell with Quantum Dot-Based Active Layer

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Quantum dot solids are known to be perspective materials for photovoltaic applications due to their unique properties. They combine strong light absorption in a wide range from UV to near-IR and relatively cheap production methods with improved charge carrier transport characteristics and lower exciton binding energies, compared to disordered organic semiconductors[1]. Lower exciton binding energies and larger exciton diffusion lengths allow for remarkable photovoltaic performance even in single-layer structure (without heterojunction)[2]. Earlier we proposed an analytical model for the J-V characteristics of such device which takes into account both exciton transport and dissociation characteristics together with hopping mechanism of charge transport[3]. However, the experimental fill factor and power conversion efficiency values of the cell could not be reproduced within that approach. Here, we propose the modification of the latter model, which takes into account the dissociation of the excitons not only in the bulk of the quantum dot active layer, but also at the layer interfaces within finite time. This modification provides better agreement with the experimental data and gives the opportunity for more careful investigation of the physics of the exciton dissociation.

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Application of Theoretical and Experimental Structural Methods to Study Macrocycles for Organic Electronics

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The increasing interest in metal complexes of porphyrins, porphyrazines and their analogues is due to the fact that these compounds demonstrate examples of their successful application for gas-phase transport in order to obtain films for various purposes, up to the formation of films of high-temperature superconductors. Their distinctive feature is that they not can only be used as volatile components for deposition of a metal layer on the surface of a semiconductor, but also exhibit outstanding semiconducting properties. Structural studies of complexes with metal ions can make it possible to analyze the influence of the nature of the metal atom on the electronic and geometry structure of ligands, to obtain information about the nature of the chemical bond between the metal and the ligand and to identify trends in changes in the covalent and ionic components of bonding.

In this work, an experimental and theoretical study of the geometric and electronic structure of molecules of macroheterocycles was carried out in order to establish and theoretically explain the general patterns in their structure, as well as expand reference information. For a comprehensive study of the structure and energetics of macroheterocyclic compounds, a complex of theoretical and experimental methods was used.

Studies of sublimation processes of cobalt hemiporphyrazine, octapropylsubstituted porphyrazine complex with silicon difluoride and ethioporphyrinate-I of silicon difluoride was performed. The study was carried out using a magnetic mass spectrometer MI-1201, modified for thermodynamic studies. The enthalpies of sublimation were determined using the Knudsen effusion method with mass spectrometric control of the vapor composition.

The structure of free molecules of ethioporphyrinate-I of silicon difluoride was determined by gas electron diffraction. Electron diffraction studies are of particular importance due to the fact that the resulting molecular structure is free from collective interactions, which makes it possible to establish with high reliability the fine details of the geometric structure of molecules necessary for reliable prediction of gas-phase processes.

An important component of the studies carried out is the theoretical determination of the geometric and electronic structure of macroheterocyclic compounds using high-level quantum chemical calculations, which made it possible to determine the effect of substituents on the structure and spectral properties of these compounds. Quantum-chemical calculations for a number of complexes with macroheterocyclic ligands were performed: porphyrazine complexes with silicon(IV), germanium(IV), tin(IV) and lead(IV) $XPzY_2$ (X = Si, Ge, Sn, Pb; Y = F, Cl, Br, OH), the octa(4-propylphenoxy)phthalocyanine complexes with Al(III), Ga(III) and In(III). In order to compare porphyrazine complexes $XPzY_2$ with porphyrin complexes XPY_2 the quantum chemical calculations for XPY_2 (X = Si, Ge, Sn, Pb; Y = F, Cl, Br, OH) have also been performed. The structures of dimeric forms of 21–thio, 21-oxa, and 21.23-dithioporphyrins have been optimized using quantum chemical calculations to study the nature of intermolecular interactions and the influence of aggregation on the optical properties of macroheterocyclic compounds.

This work was supported by RSF (project № 24-73-10107).

Influence of Semiconductor Layer Thickness on The Operational Properties of Electrolyte-Gated Field-Effect Transistor

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An electrolyte gated organic field-effect transistors (EGOFET) architecture includes an organic semiconductor (OSC) deposited between the source and drain electrodes, an electrolyte solution located on the OSC surface, and a gate electrode placed in contact with the solution. When voltage is applied to the electrode immersed in the electrolyte, electric double layers (EDL) are formed at the boundaries of the electrolyte-gate electrode and the electrolyte-organic semiconductor, which leads to electrostatic polarization of the organic semiconductor and, ultimately, to modulation of the current in the channel. Due to high capacitance of the EDLs, a significant field-effect current appears under a gate bias as low as 0.5 V, allowing sensing operations with different analytes, dissolved in liquid.

One of the most perspective gas sensing technologies are based on utilization of ultrathin film (near-monolayer) organic field-effect transistors (OFETs). For layered sexithienyl films in OFETs, the charge carrier mobility rapidly increases with increasing coverage and saturates at a coverage of about two monolayers. This shows that the first two molecular layers next to the dielectric interface dominate the charge transport of OFETs. So, by varying the thickness of the OSC the sensitivity of OFET-based sensor can be controlled.

This work aims to study the influence of thickness of semiconductor layer on the operational properties of EGOFETs. Thin-film EGOFETs with different thickness of OSC layer are fabricated by Langmuir-Schaeffer or Doctor Blade techniques. The dependence of threshold voltage, current, transconductanse of EGOFETs are studied. The influence on sensor properties of EGOFET-based sensor the is assessed.

This work was supported by Russian Science Foundation (project No. 19-73-30028).

Novel Non-Condensed Acceptors Based on 4H-Dithieno[3,2-B:2',3'-D]Pyrrole and 4H-Cyclopenta[1,2-B:5,4-B']Dithiophenen,S-Heterocycles with an Ethynylene Linker for Ternary Polymer Solar Cells with an Efficiency more than 15%

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This study explore the design, synthesis and application of two non-fused ring non-fullerene acceptors, namely ECDPT-IC and EDTP-IC, featuring an ethynylene linkers between 4H-cyclopenta[1,2-b:5,4-b0]dithiophene (CPDT) and 4-(2-octyldodecyl)-4H-dithieno[3,2-b:2',3'-d]pyrrole (DTP), respectively. The incorporation of ethynylene linker is found to be effectively regulate the energy levels and molecular conformations of non-fullerene acceptors. The EDTP-IC with DTP central core exhibit higher electron mobility, compared to ECDPT-IC. The frontier energy levels of both ECDPT-IC and EDTP-IC are more aligned with PTB7-Th and also have complementary absorption. The organic solar cells based on PTB7-Th:EDTP-IC attained higher power conversion efficiency (13.35%) as compared to and PTB7-Th:ECDPT-IC counterpart (10.87 %), attributed to efficient exciton dissociation and charge transport. Further the power conversion efficiency has been improved to 15.17 % for ternary OSC, when ECDPT-IC was added to PTB7-Th:EDTP-IC binary active layer. Although the power conversion efficiency is only about 15 %, which may be due to the fact that the absorption spectra of the active layer is only limited to 850 nm. We assume that these NFR-NFAs may have potential for very efficient indoor OSCs as well as for guest component for the OSCs using wide bandgap polymer and narrow bandgap acceptor.

This work was financially supported by the RSF (grant No. 24-43-00178), spectral characterization, NMR and x-ray diffraction studies were performed using the equipment of center for molecular composition studies of INEOS RAS with the support from ministry of Science and higher education of the Russian Federation

New 5,6-Bis(6-Fluoro-9H-Carbazol-3-Yl)Naphtho[2,1-B:3,4-B']Dithiophene Containing *Π*-Conjugated Wide Bandgap Donor Polymer Synthesized via Direct Arylation Polycondensation for Ternary Non-Fullerene Organic Solar Cells

M. L. Keshtov[1*], *A.R. Khokhlov*[1], *D. P. Kalinkin*[1], *D.Y. Shikin*[1], *H. Dahya*[2,3], *S. Karak*[2], *G. D. Sharma*[3]

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The ternary active layer approach has emerged as a promising approach to further boost the power conversion efficiency of organic solar cells. In order to absorb photons from the solar radiation below 600 nm, we have designed and synthesized a new wide bandgap polymer**P(FCzNDT-DFTPhz)** consisting of strong 5,6-bis(6-fluoro-9H-carbazol-3-yl)naphtho[2,1-b:3,4-b']dithiophene and di-fluoro-dithieno [3,2-a:2',3'-c]phenazine donor and acceptor units, respectively, its optical and electrochemical properties were investigated. The **P(FCzNDT-DFTPhz)** exhibits strong absorption spectrumbelow 650 nm along with deeper HOMO energy level (-5.46 eV), which is beneficial for attaining high open circuit voltage. Utilizing **P(FCzNDT-DFTPhz)** as donor and Y6 as acceptor, the organic solar cells fabricated under ambient conditions, processed with non-halogenated solvent (toluene) attained a power conversion efficiency of 15.59 % which is higher than that for PTB7-Th:Y6 counterparts (12.98 %). When **P(FCzNDT-DFTPhz)** is incorporated intoPTB7-Th:Y6 binary active layer, the ternary organic solar cells fabricated under ambient conditions, attained power conversion efficiency of 17.36 %, which is due to the fact that**P(FCzNDT-DFTPhz)** and PTB7-Th exhibits complementary absorption spectra, increasing thelight harvesting efficiency and exciton generation rate. This leads to a simultaneous increase in short circuit current and fill factor, originated exciton utilization via energy transfer from **P(FCzNDT-DFTPhz)** to PTB7-Th, efficient exciton dissociation owing to increase D/A interfaces in ternary active layer, higher charge carrier mobilities and well-balanced charge transport, suppressed carrier recombination and fast charge extraction time and prolonged charge carrier lifetime.

This work was financially supported by the RSF (grant no. 24-43-02039 and No.-DST/IC/RSF/2024/461),

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Stable Radicals as Admixtures in The Active Layers of Organic Photovoltaic Cells

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The stable radicals, in particular nitroxide (**TEMPO**) and galvinoxyl (**Gx**) radicals (Fig.1), being doped in organic photovoltaic cells (OPCs) could tune the parameters of photocurrent generation by several possible mechanisms. Probably, one of them is magnetic interaction between spins of charge carriers with the unpaired electrons of the radicals this interaction could strongly affect the photoinduced charge separation processes. Therefore, the purpose of the study is to reveal any characteristics of the stable and light-induced radicals within the models of the active layers of OSCs by continuous wave (CW) and pulse EPR.

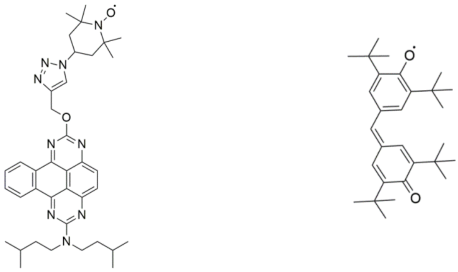

Fig. 1. Structures of the stable radicals **TAP-TEMPO** (left) and **Gx** (right)

The novel stable radical **TAP-TEMPO** was synthesized after chemical modification of tetraazapyrene heterocyclic core by the nitroxide radical **TEMPO**. The compound **TAP-TEMPO** was added into spin-coated active layers of conventional and inverted polymer:fullerene **PCDTBT:PCBM**-based OPCs. In the thin films the **TAP-TEMPO** compound covered the film surfaces as a functional interface electron blocking and/or hole transport layer[1].

The simple two-pulse electron spin echo (ESE) technique was developed to extract values of magnetic dipole-dipole interactions in aggregates of **Gx** molecules. For the **PCDTBT**:**PCBM** thin films doped by the **Gx** molecules the experimental ESE decays were successfully simulated by the following model. The magnetic interaction of the **Gx** molecules acts within the clusters of eight **Gx** molecules on the surface of a sphere with a radius of 2.0 nm[2].

This work was supported by the Russian Science Foundation (project # 23-73-00072).

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Photoconductivity in thin films of oil porphyrins

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Oil- or petro-porphyrins are a group of metal-containing tetrapyrrolic molecules found in fossil fuels and ancient sediments.[1] The metals in these molecules, mostly vanadium and nickel, are complexed with ligands whose chemical structure can roughly be divided into 3 types: *etio*- (alkanes), *dpep*- (cycloalkanes) and *rhodo* (aromatics) – Fig. 1a-c. Because of their negative role in catalytic oil refining, these complexes must be removed from the crude material, but their subsequent utilization remains a challenge for technologists.

In this work, a mixture of vanadium porphyrin complexes, VO-PPs was isolated from the asphaltene fraction of the crude oil produced in Tatarstan using innovative methods developed at IOPC RAS, Kazan. The ratio of *etio*-, *dpep*- and *rhodo*- type ligands in the resulting fine-grained powder was 23%, 58% (incl. 19% *di-dpep*) and 19% (incl. *rhodo-etio* + *rhodo-dpep*). Thin films were obtained by the thermal vacuum evaporation. The sublimation temperature T_{subl} of VO-PPs lies in a wide range of 210±40°C, which is due to the mixture composition. On most technical substrates the films are flat with a r.m.s. roughness <2.5 nm and amorphous, although T_{subl} chosen for deposition affects their optical and electrical properties.

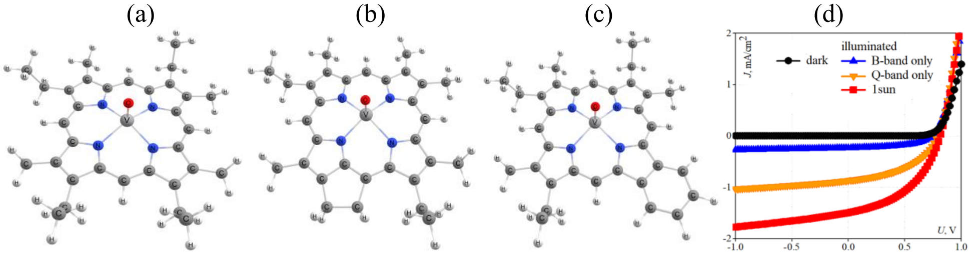

Fig. 1. Molecular structures of oil porphyrins in the form of oxovanadium(IV) complexes: (a) *etio*-, (b) deoxophyllo-erythroetio (*dpep*) and (c) *rhodo*. Dark and illuminated (various sources) *J-V* plot for the device 'glass/ITO/MoO_3/*p*-VO-PPs/*n*-Cl_6SubPc/BCP/Al'

Both planar (symmetrical) and sandwich-type photoelectrical cells with VO-PPs films were fabricated and tested.[2] DC conductivity of films is highly sensitive to lighting conditions, strictly following the profile of their narrow-band optical absorption. In contrast with pure VO-*etio* films, the ratio of the integral absorption in the range of B-(Soret) band and Q-band in the visible spectrum practically coincides with the ratio of the photoconductivity gain under filtered illumination (~15) – Fig. 1(d). Intermolecular interaction/aggregation leading to band broadening are suppressed in mixed porphyrin matrices.

By pairing VO-PPs with the porphyrin-type acceptor Cl_6SubPc, we fabricated archetypal semitransparent photovoltaic cells with planar molecular heterojunction and standard electrode buffer layers – Fig. 1(d). While photoconversion efficiency of such cells is of the order of few percent, the air stability and photovoltage are comparable to those when employing isomeric-pure *etio*-porphyrin donors (~0.8V)[2] – Fig. 1(d). Prospects for using petroleum-derived porphyrins as active materials in optoelectronic devices are discussed.

This work was supported by RSF (project № 25-73-20101).

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Design of Triphenylamine-Based Molecules with Anchor Group for Interfacial Layers of Perovskite Solar Cells

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Perovskite solar cells (PSCs) are a rapidly evolving technology, with their efficiency soaring from 3.8% in 2009 to over 25% by 2025, allowing them to compete with and even outperform traditional silicon solar cells in laboratory conditions[1]. These characteristics, combined with low-cost materials and ergonomic manufacturing methods, have made PSCs a promising photovoltaic technology. A major problem standing in the way of commercialization and scaling of PSCs is their low stability, as well as degradation during operation of the device. The solution to this problem is the use of auxiliary layers in the PSC architecture, the so-called interface layers based on organic semiconductor materials. The feature that allows such materials to effectively "treat" defects in the perovskite structure is the presence of special functional groups (anchor groups) capable of specific interactions with the perovskite material and other charge-transport layers, as well as of self-assembly. However, the variety of possible surface and volume defects in perovskite, leads to the problem of finding optimal structure of the self-assembled materials. An important part of these materials is the terminal group, which is oriented toward the perovskite layer and responsible for specific interactions with the active layer. In addition, the terminal group affects the surface properties of the film formed by the material; the combination of all properties, including optical, electrochemical, etc., has a significant impact on the efficiency and stability of PSCs and perovskite solar modules (PSMs), as we have shown previously[2,3]. Nevertheless, the selection of structural blocks for this group, as well as the search for optimal substituents in it, is currently an unexplored area of scientific knowledge.

In this work, a comprehensive study is conducted to identify a number of patterns of influence of substituents at the terminal group on the properties of compounds. For this purpose, an effective scheme of the synthetic route of a series of compounds differing in the substituent at the terminal group was developed, a set of their physicochemical properties (such as optical and electrochemical properties, thermal stability and phase behavior) was studied. The surface properties of films formed by the materials were investigated, and the influence of substituents and their donor-acceptor nature on the complex of properties of the obtained compounds was revealed. The possibility of using these materials in PSCs was assessed – for all materials, efficiency indicators of more than 20% and good stability were achieved.

This work was supported by the Russian Science Foundation (grant No. 22-19-00812-P).

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O-22

Novel Organic and Hybrid Organic-Perovskite Composite Materials for Light Emitting Application

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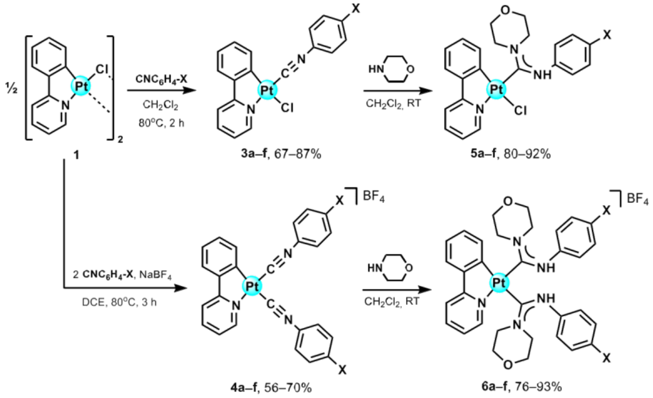
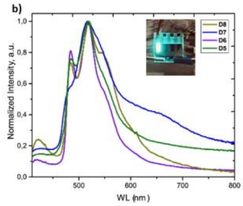
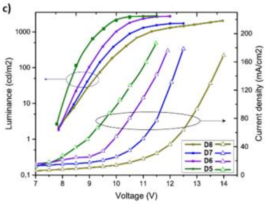
A novel series of cyclometalated platinum(II) complexes bearing acyclic diaminocarbene (ADC) ancillary ligands was designed and developed. Their photophysical properties were systematically studied through experimental and theoretical investigations. All complexes exhibit green phosphorescence with quantum efficiency up to 45% in 2 wt% doped PMMA film at room temperature. The complexes are used as light-emitting dopants for organic light-emitting diode (OLED) fabrication. The devices displayed a green emission with maximum current efficiency of 2.9 cd·A−1 and luminance of 2700 cd·m−2. These results show that this type of cyclometalated platinum(II) complex can be utilized as efficient green phosphorescent emitters.







X = NMe_2 **a**; Me **b**; Cl **c**; Br **d**; I **e**; CF_3 **f**.

In this work, we report a comprehensive study of the cyclometalated platinum complexes supported by ADC ancillary ligands, which display phosphorescence in the green spectral region. A panel of new PtII-ADC complexes was prepared via the metal-mediated coupling of various arylisocyanides with amine nucleophile (morpholine). The ADC ligands are modified with electron-donating (C_6H_4-4-NMe2, C_6H_4-4-Me) or electron-withdrawing (C_6H_4-4-Cl, C_6H_4-4-Br, C_6H_4-4-I, C_6H_4-4-CF_3) aryl groups. Our investigation revealed that substituent changes on the aryl in the ADC ancillary ligand can affect emission quantum yields and excited state lifetimes without any significant changes of the emission maxima and spectral profiles. Also the design of class of modular polyfluorene (PF) copolymer with 4-hydroxyphenyl-, diethylamino- and diethoxyphosphoryl- groups to stabilize perovskite nanocrystals (NCs) will be discussed. Resulting polymer/NCs composite showed efficient Förster energy transfer (FRET) from PF to NC with green photoluminescence (PL). We also found that the NCs composite studied here can be used as an effective emissive layer in LED due to the strong interaction between polymer host and perovskite NCs providing an efficient charge transfer from the PF matrice to the NC emitter. The fabricated LED show excellent performance with a highest current efficiency of ~25.2 cd A–1.

This work was supported by State assignment No. FSER-2025-0011

Poster presentations

Features of Crystallization in Solutions of 4,7-Diphenyl-2,1,3-Benzothiadiazole and Its Derivatives with Terminal Alkyl Substituents

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Among short donor–acceptor molecules with a central 2,1,3-benzothiadiazole fragment, 4,7-diphenyl-2,1,3-benzothiadiazole (**P-BTD**) is one of the most effective luminophores with high thermal and photochemical stability. Triclinic crystals (P-1, Z=4) are formed from solutions under slightly nonequilibrium conditions, the fluorescence quantum yield of which reaches 50% (λ_{max}=493 nm).[1] However, under strongly nonequilibrium conditions of deposition of the substance on the substrate (spin-coating, PVD), the formation of continuous layers is not observed due to the emergence of several polymorphic phases that segregate over time. The addition of terminal substituent groups allows for the variation of the physicochemical characteristics of the compounds in order to improve the crystallization characteristics and physical properties of the crystals. The report presents the results of a study of the features of crystallization from solutions, structure, some thermodynamic and fluorescent properties of **P-BTD** crystals and its derivatives with terminal alkyl substituent groups (Fig. 1).

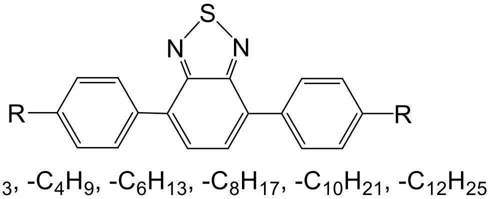

Fig. 1. General structural formula and abbreviations of the investigated compounds: R = -H (**P-BTD**); $-CH_3$ (**Me-P-BTD**); $-C_4H_9$ (**C4-P-BTD**; $-C_6H_{13}$ (**C6-P-BTD**); $-C_8H_{17}$ (**C8-P-BTD**); $-C_{10}H_{21}$ (**C10-P-BTD**); $-C_{12}H_{25}$ (**C12-P-BTD**)

This work was supported by Russian Science Foundation (project № 22-13-00255-П), https://rscf.ru/en/project/22-13-00255/.

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P-2

A Two-stage Heating Mode for Thermomechanical Muscles Testing

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A composite material that uses a liquid-gas phase transition under heating conditions was pioneered in[1]. The foamed structure of the composite is formed by the addition of a pore-forming agent ethanol, to the curing silicone rubber. Initially, ethanol is mixed with the rubber, and during the cure it is released into a separate phase in the volume of the composite, forming spherical pores filled with ethanol. Heating such a composite above the boiling point of ethanol (78.4°C) leads to its evaporation in the pores and, accordingly, to the expansion of the composite sample.

The rejuvenation, i.e. the recovery of the composite functionality by the refilling its pores with ethanol was shown in[2], the use of others alcohols C1-C4 was shown in[3]. In this work, the composite was rejuvenated with a solution of benzoic acid in ethanol. The pressure of saturated vapors of the acid is high (1 kPa at 20 °C) and when the composite is heated, its sublimation will increase the strain of the sample.

To demonstrate the effect of the sublimating agent on the deformation of the composite, a two-stage heating was proposed. At the first stage (8 W), the sample was heated to the temperature 15 °C higher than the boiling point of ethanol allowing it to evaporate, and at the second stage (10 W), the temperature rose to 120 °C, but significantly lower than the boiling point of benzoic acid (249 °C). The strain was recorded using the PARUS (ISPM) device. The dependence of the composite strain on time during testing in a two-stage mode is presented below.

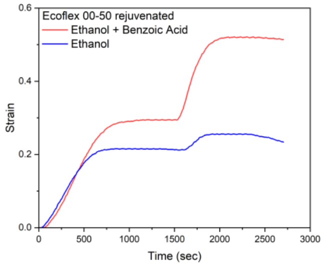

Fig. 1. The strain for two-stage mode heating (8 W + 10 W) of the rejuvenated composite

When heated, ethanol and benzoic acid vapors diffuse through the silicone matrix outside the composite sample, thus limiting the possibility of reusing the composite.

This work was supported by the Russian Science Foundation (project № 19-73-30028-P).

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P-3

New Triazine -Based Molecules for Organic Electronic Devices

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The development of novel organic materials with tunable optoelectronic properties is crucial for advancing the performance of organic electronic devices, such as organic light-emitting diodes (OLEDs) and organic photovoltaics (OPVs).

BTD derivatives serve as effective electron-acceptor units, improving the electronic characteristics of organic materials used in OLEDs and OPVs.[1] A specific BTD derivative demonstrated solvatochromism and acted as a p-type semiconductor in OFETs[2], achieving hole mobilities of up to 0.1 cm²/V·s. Devices using triazine derivatives have shown power conversion efficiencies exceeding 16% and electron mobilities of 8 cm²/V·s, indicating their potential in high-performance organic electronics.[3]

This study reports the design, synthesis, characterization, and application of new molecules based on a triazine core coupled with a benzothiadiazole (BTD) unit, designed to exhibit desirable electronic and optical characteristics.

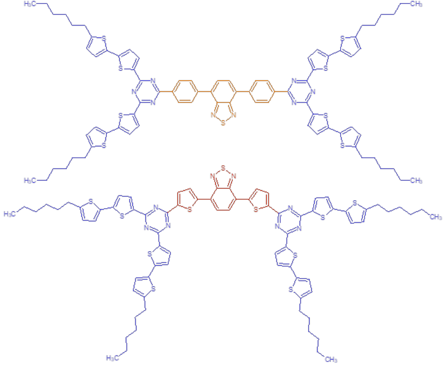

Fig. 1. The structure of new molecules based on triazine and BTD

The synthesized molecules, designated as 2T-TRZ-Ph-BTD and 2T-TRZ-T-BTD, were carefully designed to leverage the electron-withdrawing properties of the triazine and BTD moieties, aiming to enhance electron transport and promote intramolecular charge transfer (ICT). The synthesis route involved reactions of bromination, Suzuki, Miyaura, Grignard, Kumada followed by purification by standard methods such as recrystallization and column chromatography. The resulting material was characterized by NMR spectroscopy and mass spectrometry, confirming its chemical structure and purity.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation, State contract FFSM-2024-0003.

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P-4

Anion Effect on Modulation of Synaptic Properties of Organic Biocompatible-Ionogel Electrolyte Neuromorphic Transistors for Deep Neural Networks

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Organic neuromorphic transistors, with their low power consumption, high tunability, readily available materials, and low cost, demonstrate significant potential for developing novel brain-inspired, energy-efficient, and highly parallel non von Neumann computing systems.[1]

Electrolyte-gated organic field-effect transistors (EGOFETs) based on ionogels offer long-term stability, biocompatibility and low power operation. High capacitance of electrolytes reduces driving voltages allow these devices simulate synaptic characteristics via ion diffusion-induced potential changes, such as excitatory postsynaptic current (EPSC), short-term synaptic plasticity (STP), paired-pulse facilitation (PPF), and adaptation.

This study investigates the anion effect on modulation of synaptic properties of organic biocompatible-ionogel electrolyte neuromorphic transistors for deep neural networks. We developed a formulation of ambient stable ionogels based on scope of ionic liquids and EGOFETs using P3HT as the organic semiconductor were investigated. The correlations were established between anions structure, ionic conductivity, diffusion properties and synaptic response parameters, including average current decay time (τ_{avg}), EPSC amplitude, and PPF index (Fig. 1).

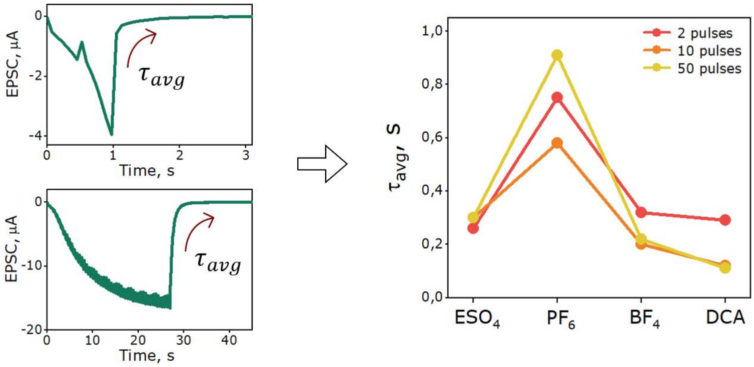

Fig. 1. PPF and EPSC for EGOFETs (left) and average current decay time (τ_{avg}) for different ion gel anions (right)

Overall, ionogel electrolyte composition was found to be crucial for EGOFETs neuromorphic properties modulation. Variation of anions structure in EGOFETs offering a versatile platform for application in artificial synapses and neuromorphic computing.

This work was supported by the Ministry of Science and Higher Education (project No FSUS-2021-0014).

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High-Vacuum Sublimation of Organic Semiconductor Materials for OLEDs

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In the inorganic LED industry, semiconductor materials with a purity of 99.99% (4N) and higher are a strict standard due to the high sensitivity of optoelectronic performance to impurities[1]. However, in the field of organic light-emitting diodes (OLEDs), such mandatory purity requirements are often overlooked, despite the crucial role that material quality plays in device efficiency, lifetime, and reproducibility[2].

In this study, we present a practical approach to the purification of organic semiconductor materials—both hosts and dopants—using a custom-built high-vacuum sublimation system. The apparatus allows precise control over temperature (up to 400°C) and pressure (down to 10^{-6} mbar), enabling efficient removal of low-volatile and high-volatile impurities without decomposition of the target compounds.

We demonstrate the purification of several commonly used OLED materials and compare their photophysical properties before and after sublimation. The results show significant improvements in purity, verified by spectroscopic and chromatographic methods. Our work highlights the importance of material purification for organic electronics and provides a scalable and accessible method for improving the consistency and performance of organic semiconductors.

Fig. 1. Photo of a comparison between the same typical semiconductor compound before and after sublimation purification

This work was supported by Ministry of Science and Higher Education of Russian Federation (project FFSM-2025-0004).

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Impact of Organic Light Emitting Diodes Structure on The Charge Carrier Recombination Profile

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One of the main problems of modern organic light-emitting diodes (OLEDs), especially blue ones, is their insufficient lifetime in operating conditions. One of the key reasons for OLEDs' degradation is associated with the degradation of the organic emission layers and their interfaces mainly within the electron-hole recombination zone, where the exciton density is high. As a result, the energy density is high as well, which can result in a high probability of degradation.[1] The spatial profile of the recombination rate within the emission layer is determined mainly by energy barriers at the interface of adjacent layers.[2] In this work, using drift-diffusion numerical model with direct recombination approximation, the optimization possibilities of the charge carrier recombination rate spatial distribution by selection of optimal transport layer materials have been investigated.

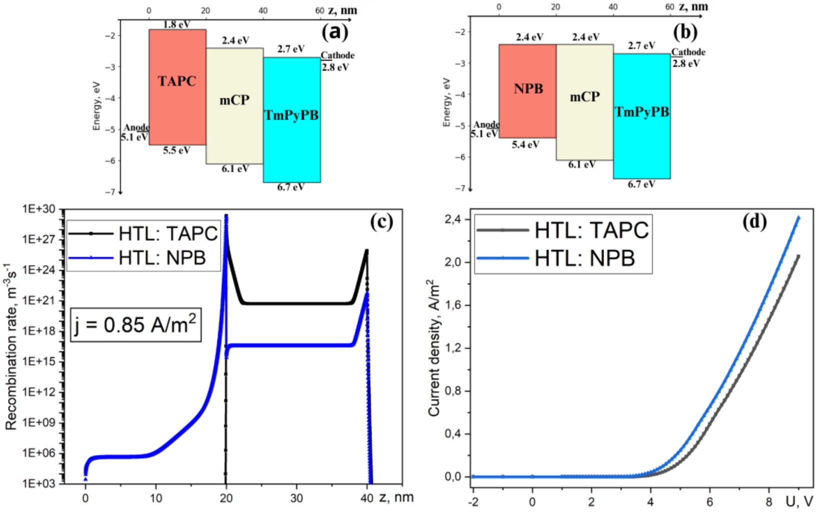

Fig. 1. OLED energy diagrams (a, b), spatial distributions of the charge carrier recombination rate at current density of j = 0.85 A/m^2 (c) and current-voltage characteristics (d) for two hole transport layers, TAPC and NPB, and the same emission and electron transport layers

Different recombination profiles of charge carriers are observed for two structures with NPB and TAPC hole-transport layer materials (figure 1, c). In that way, by choosing the optimal combination of materials, it is possible to shift the recombination zone from the interface to the center of the emission layer and increase the operational stability of the device.

The authors wish to express their gratitude to Luponosov Yu.N. for providing data on the materials' properties. This work was financially supported by Ministry of Science and Higher Education, state assignment FFSM-2025-0004.

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Creation And Research of Luminescent Compositions with Improved Characteristics for Light-Conversion Photoresists

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Wavelength-converting photoresists (WCPRs) are promising materials for enhancing the performance of micro- and nanolithographic processes, including OLED structures in high-quality displays.[1] This work presents an approach to the development and investigation of luminescent compositions (LCs) with enhanced properties for application in WCPRs, aimed at improving their efficiency and extending the spectral range of sensitivity.

The objective of this study is to engineer LCs exhibiting high photoluminescence quantum yield, stability, and compatibility with the oligomer matrix of the photoresist. Vin-Si-TPA-BTD and Vin-Si-DPA-Antr were selected as luminophores. The synthesis of the LCs was carried out using photo-curing of an oligomer with luminophore in solution employing photoinitiator of polymerization: benzophenone.

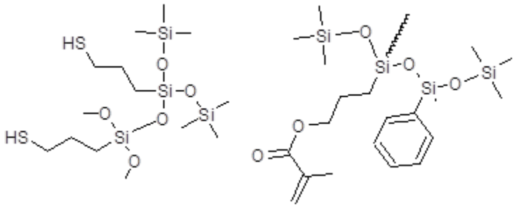

Fig. 1. Oligomers with terminal thiol and acrylate groups

The synthesized LCs were characterized via absorption and photoluminescence spectroscopy. The results showed that the fluorescence in the films is similar in shape to the solution data, for the green film the fluorescence maximum coincides with the solution one, but for the red film the maximum is shifted to a shorter wavelength region by 11 nm (615 and 605 nm, respectively), and the quantum yield was 40% for both films.

The developed LCs exhibited enhanced characteristics and demonstrate a promising potential for application in WCPRs, enabling improved efficiency and expanded capabilities of photolithographic processes.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation, State contract FFSM- 2025-0004.

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Modeling The Behavior of Circular Dielectric Elastomer Actuators

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Dielectric electro-active polymer technology holds promise for enabling lightweight, energy efficient, and scalable dielectric elastomer actuators (DEAs). The circular DEA actuator configuration (also known as cone or diaphragm actuator) in particular shows potential in applications such as pumps, valves, micro-positioners and loudspeakers. For a quantitative prediction of the actuator behavior as well as for design optimization tasks, material models which can reproduce the coupled electromechanical behavior inherent to these actuators are necessary. A complete model of the DE material and actuator system components is required to improve the design process and reduce the time and cost of prototyping devices using DEAs. In addition, the model is intended for use in the design of a model-based feedback control. The model must take into account the visible damping and viscoelastic effects of the DE material, so it can describe higher frequency applications such as pumps and valves. This paper presents a model of the actuator with simulations that show good agreement with experimental results for static operating conditions.

The model relates the applied voltage (*input*) to the vertical displacement (*output*). Here, the static response is taken into account by the model. The model output is the vertical displacement of the center of the DE (with the weight on). For this reason, the static equilibrium equation of the force on the vertical axis yields the equilibrium equation.

$$mg - F_{DE} \cdot \sin\theta = 0$$

Assuming that the deformed DEA's geometry is a truncated cone, the DE is incompressible, and decomposing the radial stress into its elastic (Mooney-Rivlin solid) and electrostatic (Maxwell stress) components, the latter can be written as:

$$mg - \frac{4\pi r z_0 C_{10} x}{l_0}\left[\left(1 - \frac{l_0^6}{(l_0^2 + x^2)^3}\right)\left(\frac{C_{01}}{C_{10}} + 1 + \frac{x^2}{l_0^2}\right) - \frac{\varepsilon\varepsilon_0 V^2}{2C_{10} z_0^2}\right] = 0$$

where ε_0 is the free-space permittivity (8.85×10^{-12} F m^{-1}), ε is the dielectric constant, C_{10} and C_{01} are the Mooney-Rivlin parameters, z_0 is the initial thickness, l_0 is initial length, r is the radius, V is the applied voltage.

The preliminary results showed an excellent match between the model and the experimental data at the induced voltage range of 0–6 kV (see Fig. 1).

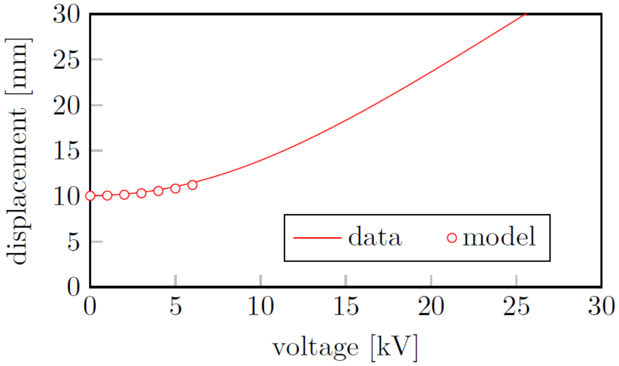

Fig. 1. Vertical displacement of the circular DEA as a function of applied voltage

This work was supported by RSF (project № 19-73-30028-P).

Theoretical Development of Diboraanthracene TADF Luminophores for Green OLEDs

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The development of organic light-emitting diodes (OLEDs) remains a relevant research area. The key tasks in this area at the moment are to increase the efficiency and stability of OLED-based devices. A possible solution to the identified problems could be the transition to the concept of third-generation OLEDs based on luminophores with the effect of thermally activated delayed fluorescence (TADF), the physical behavior of which provides the opportunity to increase both the efficiency of the device and its durability.

Relatively recently Cheng's group developed a new class of TADF-luminophores based on diboraanthrace core.[1,2] It was shown that OLEDs based on such compounds demonstrate high values of external quantum efficiency with low roll-off and promising lifetimes. However, their color characteristics (including green **tBuCzDBA**) do not meet modern standards.

In order to obtain a green luminophore with improved color characteristics, we decided to preliminarily conduct a comprehensive modeling based on the principles of molecular design (Fig. 1). It was determined that a small hypsochromic shift of the spectrum relative to the reference **tBuCzDBA** by 10-30 nm is necessary to improve the color coordinates. Taking this into account, we proposed 13 structures related to **tBuCzDBA**, the substituents in which potentially introduce small changes into the position of the energy levels. The positions of their luminescence bands were predicted using the time-dependent density functional theory method at the PBE0/def2-SVP/CPCM level of theory. The modeling results were corrected using a linear regression model built on the training set. Following the requirement of a small hypsochromic shift, we selected 4 compounds from the proposed series, for which we additionally predicted the ΔE_{ST} gap and the position of the frontier orbitals. The predicted values support the TADF effect in such systems and the possibility of their employment in devices with an architecture similar to that of the **tBuCzDBA**-based.

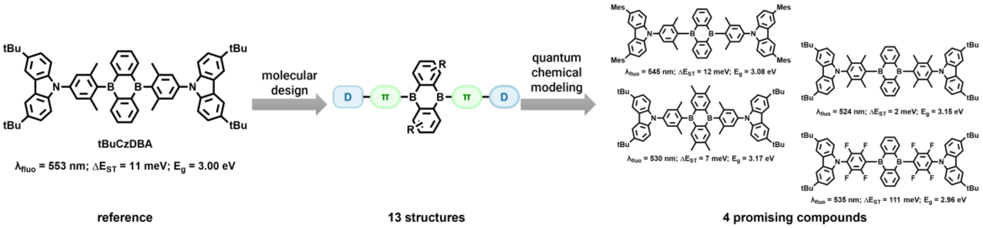

Fig 1. Design route for green luminophore

This work was supported by the Russian Ministry of Science and Education (project no. FFSM-2024-0003).

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P-10

Development of Modified PDMS/MQ Composite as Dielectric Elastomers Actuators

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Polysiloxanes are widely used in many areas, such as the cosmetic industry, electronics, biomedicine, artificial muscles, etc.[1,2,3] Such a variety of applications is due to the unique properties of polysiloxanes: the ability to work in a wide range of temperatures, weather resistance, inertness, hydrophobicity, chemical resistance, low dielectric constant, etc. To expand the properties of PDMS, various modifying groups are introduced into the main chain.[4,5] This paper will present the results of obtaining elastomer compositions based on high-molecular polydimethylsiloxane, modified linear and MQ copolymers (Fig. 1), obtaining dielectric elastomer attractors based on them and studying the conditions of their activation.

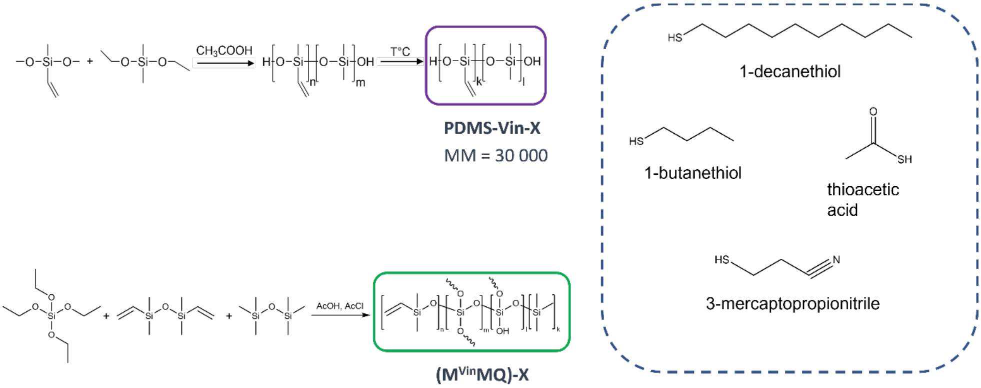

Fig. 1. Obtaining modified PDMS and MQ-copolymers

The analysis of the products was carried out using a combination of physical and chemical research methods (NMR spectroscopy, GPC, DSC, IR). The work investigated the influence of the ratio of the components of the compositions, as well as the temperature of their curing on the properties of the resulting films.

This work was supported by RSF (project № 19-73-30028).

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Synthesis and Study of The Properties of Host-Materials for the Emitting Layer of OLED

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It is difficult to imagine the development of modern digital, manufacturing and robotic technologies without the use of organic light-emitting diodes (OLEDs). OLED-based devices combine high brightness and contrast with a relatively simple production method. The most important component of an OLED is the light-emitting layer, which usually consists of the "host" and the added "dopant". The ability to select the optimal molecular structure (molecular design) of the light-emitting layer allows for improving the color, brightness stability and efficiency of devices, as well as avoiding the concentration quenching of luminescence characteristic of most phosphors.

The work presents methods for synthesizing two matrices with promising application in the emitting layer of OLEDs. The synthesis of the NAPPT matrix based on triphenyltriazine and naphthylanthracene was carried out according to the Suzuki reaction from previously obtained organoboron and bromine derivatives in the presence of a palladium catalyst[1]. To obtain highly pure compounds, further purification from the catalyst and impurities was carried out by column chromatography on silica gel with mandatory sublimation. The purity and structure of the precursors and the final product were determined by GPC (gel permeation chromatography) and NMR ^{1}H spectroscopy.

Different structures of OLED cells based on the obtained host-materials were manufactured and their properties were studied. Measurements of the current-voltage characteristics, OLED electroluminescence spectra were carried out, and OLED parameters were calculated. The results one of the studied cells showed: maximum electroluminescence at 467 nm, FWHM = 63 nm, color coordinates CIE (x; y) (0.163; 0.303), maximum IEC = 1.53% and efficiency = 1.11%, as well as a maximum brightness of 5255 cd/m2 at a current density of 744 mA/cm2. The obtained data indicate the prospects for using synthesized matrices in OLEDs.

This work was supported by RFBR (project FFSM-2025-0004*).*

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P-12

NIR OLED Based on Ytterbium Complexes with Schiff Bases

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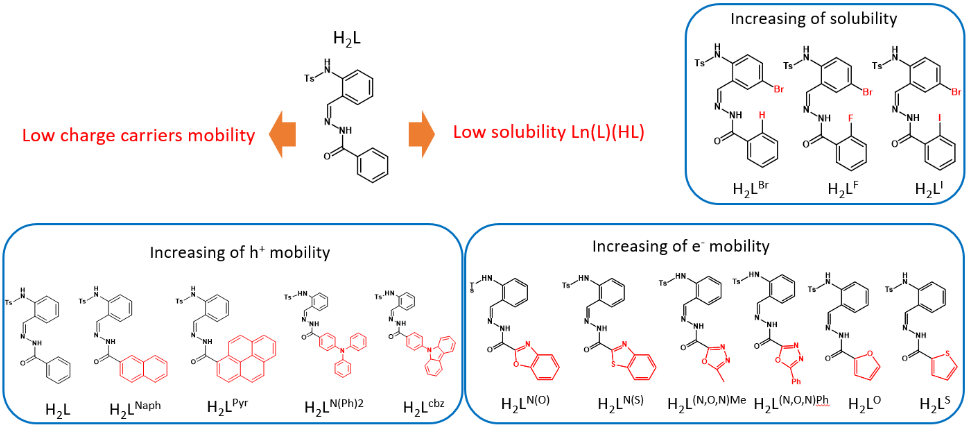
Near-Infrared (NIR) Organic Light-Emitting Diodes (OLEDs) are promising as radiation sources for wearable devices (e.g., pulse oximeters, health monitoring sensors), lab-on-a-chip microfluidic sensing systems, and related applications. One of the key parameters determining the accuracy of analyte concentration detection is the emission bandwidth of the light source absorbed by the analyte. Because it is directly related to the measurable concentration range and, consequently, to sensitivity. Lanthanide coordination compounds (CCs) combine narrow luminescence bands (10–15 nm FWHM) characteristic of lanthanide cations with broad opportunities for tuning the physicochemical properties of the organic ligand. Among all NIR-emitting lanthanide cations, ytterbium (Yb^{3+}) exhibits the highest efficiency, with photoluminescence quantum yields (PLQY) reaching several percent. This makes NIR OLEDs based on Yb^{3+} CCs particularly attractive for further investigation.



In this study, a series of lanthanide CCs featuring substituted Schiff bases as emissive layers (EML) in OLEDs was investigated. Specifically, halogen-substituted Schiff bases were studied for their enhanced solubility even in the form of Yb(L)(HL) complexes, enabling the formation of high-quality thin films for EML. Naphthyl- and pyrenyl-substituted ligands demonstrated improved electron transport due to the extended π-conjugated systems within the ligand structure. Electron-donating (di(phenyl)aminophenyl-) and electron-accepting (phenyl(oxadiazolyl)- and methyl(oxadiazolyl)-) hydrazone substituents were introduced to improve charge carrier transport within the EML bulk. It was shown that the introduction of even a single halogen substituent (F or Br) significantly increases solubility in EtOH or THF, enabling high-quality EML film formation and enhancing the external current efficiency (ECE) of the OLED by a factor of two—from 50 to 100 µW/W. The combination of an electron-donating and an electron-accepting ligand in a heteroleptic CC led to a 25% improvement in OLED efficiency compared to a mixture of two homoleptic CCs, from 110 to 140 µW/W. Furthermore, optimization of the OLED heterostructure, particularly the charge-transport layers, for a Yb^{3+} CC bearing a naphthyl-substituted Schiff base enabled an ECE of up to 441 µW/W, which, at the time of publication, was among the highest reported.

P-13

Baseline Drift Correction for OFET-Based Gas Sensors

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In recent years, gas analysis systems based on organic field-effect transistors (OFETs) have found wide application in environmental monitoring and related fields.[1,2] However, one of the key limitations affecting the accuracy of quantitative analysis in such sensors remains baseline drift[3] — a slow, systematic shift of the output signal caused by external factors, recovery processes, or sensor material degradation. To address this challenge, this work explores the use of software-based correction using the asymmetrically reweighted penalised least squares (arPLS) algorithm.[4]

The study focuses on the processing of experimental data acquired from OFET sensors during test cycles involving various concentrations of toxic gases. The arPLS algorithm provides iterative baseline correction, enabling improved reproducibility and enhanced feature extraction from sensor signals (see Fig. 1). Special attention is given to investigating the influence of the smoothing parameter λ on the outcome of the correction and on its robustness with respect to different sensor datasets.

The discussion highlights specific aspects of arPLS application for different classes of OFET devices, as well as its current limitations and future prospects for automated sensor data analysis. The results may inform further development of data-driven approaches for signal processing in gas sensor systems.

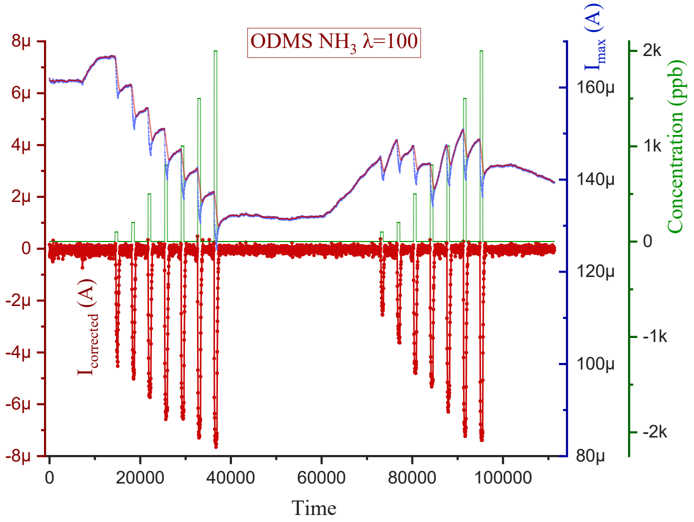

Fig. 1. Comparison of the raw and corrected OFET sensor signal after arPLS application, λ = 100

This work was supported by Russian Scientific Foundation (project No. 19-73-30028-P).

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Influence of Intermolecular Interactions on The Electronic Absorption Spectra of SiF_2-Etioporphyrin

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It is well-known that the photoconductivity of molecular films depends greetly on how the molecules are packed relative to each other and/or to the current flow[1]. Intermolecular interactions of intensively absorbing dye molecules, like porphyrins, are well reflected in electronic absorption spectra, which make their modeling an interesting and important task.

In this work, we tested various geometries of the solid-state aggregates of SiF_2-etioporphyrin, an efficient donor molecule in PHJ-based photovoltaic cell, taken from single-crystal X-ray analysis. Simplified time-dependent density functional theory (sTDDFT) in combination with PBEh-3c calculations was used for simulation of electronic absorption spectra of monomeric SiF_2-etioporphyrin and their aggregates. The electronic spectra of the monomer were simulated with accounting for the solvent (CPCM method, chloroform). The results were compared with the experimental spectra of dilute solutions and thin films.

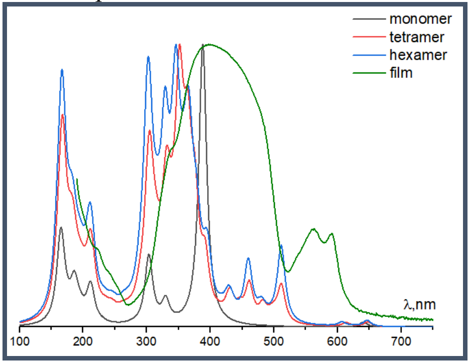

Fig. 1. Simulated spectra of SiF_2-etioporphyrin in monomeric and variously aggregated forms

Theoretical curves for mono-, tetra and hexamers are shown in Figure 1, along with the experimental spectrum of a thin film. The best agreement was obtained when the aggregate consisted of stacks arranged in a line – Figure 2. This suggests that in the case of SiF_2-etioporphyrine, the interactions between the target and all surrounding molecules in the crystals, not just those in the stack, should be considered when performing DFT calculations.

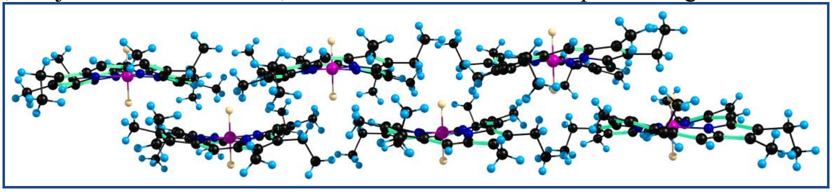

Fig. 2. The relative position of SiF_2-etioporphyrine molecules in a hexamer

This work was supported by RSF (project № 24-73-10107).

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Azolyl-Containing Luminescent Materials Based on *Ortho*-Carborane

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V.N. Charushin[1,2], *O.N. Chupakhin*[1,2]

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Currently, organic fluorophores are finding application as working components of molecular electronics devices. One of the main criteria for creating working components of these devices is their thermal stability, therefore the introduction of various substituents into the structure of the molecule is one of the important tasks in this area.

The introduction of an *ortho*-carborane fragment into the fluorophore structure affects not only thermal stability, but also their electrochemical and photostability. In addition, the electronic and dimensional structure of this substituent allows for tuning of the photophysical properties of the desired compounds.

In this work, methods and technology for obtaining molecular systems based on various azoles and *ortho*-carborane are developed. The photophysical properties of the obtained fluorophores were studied both in solvents of different polarity and in solid form. The obtained compounds are of interest in the design of new organic light-emitting diodes, semiconductors and other molecular electronics devices.

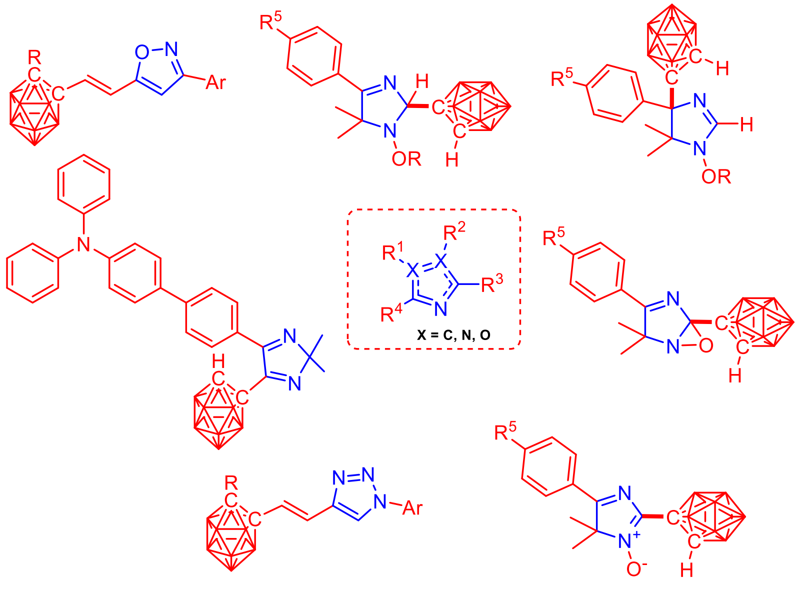

Fig. 1. Ortho-carboranyl derivatives of azoles

Molecular Design of Polymer Materials Composed of Polyimide Matrix and Azochromophores Guests for Electrooptical Applications

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Materials with quadratic nonlinear optical (NLO) responses to applied high-intensity electric field have great potential for creating optoelectronic devices. The undoubted advantage of such materials compared to inorganic analogs is significantly higher NLO characteristics, good thermal and photostability, etc. Therefore, the development of such materials is a burning task. Traditional organic NLO materials consist of a polymer matrix with embedded chromophores (conjugated molecules with a large dipole moment and first hyperpolarizability, which determines the electrooptical (EO) response of the material at the molecular level). An important feature of such materials is the ability to "tune" the EO and other properties (for example, thermal stability) by selecting polymer matrices and guest chromophores that meet specified requirements. Therefore, the search for new structural components for creating EO materials is one of the important tasks in this field of materials science.

In this study, the structure and EO properties of new composite materials based on linear polyimides (PI-L) and chromophores-guests (DO_3 and DEA-AB-TCV) (Fig. 1) were studied using molecular modeling[1].

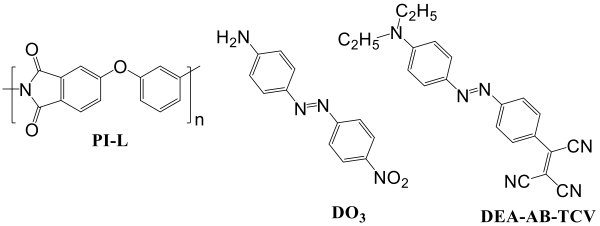

Fig. 1. Structures of the studied polymer matrix and chromophores-guests

The glass transition temperatures of the pure polyimide PI-L and composite materials based on it were theoretically calculated; the effect of introducing chromophores-guests on the glass transition temperature (T_g) of the material was considered in the course of modeling in an applied electric field. The order parameter characterizing chromophores alignment in the model composite materials was estimated.

It was found that with an increase in the weight content of chromophores DEA-AB-TCF from 10 to 30 wt.%, the T_g of the material decreases by about 50 K. However, material containing the DO_3 chromophore, even at a 10 wt.% content, the T decreases by approximately 30 K compared to the Tg of pure PI-L. For composites, the modeling of the poling stage - the orientation of chromophores in the applied electric field - was carried out. It was found that the optimal poling temperature is slightly higher than T_g, and the field strength is about 500 V/µm.

This work was supported by the Russian Science Foundation (project № 24-73-00084).

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Geminate Pair Separation Probability in Organic Semiconductors: The Effect of Disorder and Energy Nonequilibrium (A Monte Carlo Study)

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To construct an efficient photovoltaic device based on organic disordered semiconductors (ODS), studying the photogeneration process and transport characteristics of charge carriers (electrons and holes) is necessary. Due to the structural (off-diagonal) disorder and the energy disorder it induces, the carrier transport is solely via hopping between localized states. The permittivity of ODS is usually small, therefore, a geminate pair (GP, also known as CT state) is formed after primary exciton separation, which is bound by a strong Coulomb interaction. The probability of GP separation (overcoming the Coulomb barrier) determines the efficiency of the device. For an analytical description of this process, the Onsager model is often used, which significantly underestimates the separation probability in the low-temperature region compared to the experimental results and Monte Carlo (MC) simulation. This is due, for example, to the issues that the classical Onsager model does not account for the effect of disorder as well as does not consider strongly nonequilibrium (dispersive) transport at short separation times (when jumps occur predominantly downwards in energy). The modification of the Onsager model, in which the values of effective initial separation and effective temperature are introduced, describes the temperature dependences more successfully[1]. The MC method is an important tool for theoretical modelling of electron transport in ODSs, predicting the characteristics of novel materials and verifying analytical models. Lately, MC modelling has been applied to investigate the effect of Gaussian energy disorder on the photogeneration internal quantum yield[2] and to estimate the effect of off-diagonal disorder on charge mobility and efficiency of GP separation (however, under some special assumptions)[3]. In the present study, we model the dependence of the geminate pair separation probability on the value of Gaussian disorder, temperature, and applied electric field. Particular attention is paid to how both the equilibration degree of the initial (following the decay of a primary exciton) energy distribution of mobile carriers and the radius of carrier localization affect the photoseparation. These parameters can vary for different materials, and their influence is quite poorly investigated. It is shown, in agreement with the previous work[i], that the separation probability is much higher than predicted by the Onsager model at low temperatures. The temperature and field dependence of the GP separation efficiency is determined by the degree of carrier localization. In the case of initial quasi-equilibrium, depending on disorder and degree of localization, the separation probability can be both higher and lower than the result of the Onsager model. As far as weak localization is concerned, the impact of long jumps from low-lying states leads to a drastic drop in the separation efficiency with decreasing temperature. Besides that, an analysis of the effect of off-diagonal disorder (in addition to energy disorder) and the thickness of the ODS layer on the GP separation probability is performed.

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New Diindolophenazine-Based Fluorophores with Highly Efficient Blue Electroluminescence

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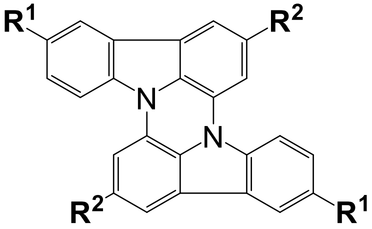
The development of reliable blue OLEDs with high efficiency and stability is still an Immediate task, since their characteristics largely lag behind the green and red ones. Thus, significant efforts have been made to improve the performance of blue OLED displays. Recently, due to conceptual advances in molecular design, sky-blue OLED displays based multiresonance effect materials as emitters or sensitizers for fluorophores have been rapidly developing both in terms of efficiency and service life. In this work, we obtained new fluorophores symmetrical and asymmetrical structures based on diindolophenazine cores for blue OLEDs.



This work was supported FFSM–2025–0004.

P-19

New Method of Determining Charge Carrier Mobility in Thin Layers of Organic Crystals Using Time-of-Flight Technique

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The time-of-flight (TOF) experiment is a common method for determining material mobility $\mu = V/F_0$, where V is the drift velocity of the charge packet and F_0 is the constant and uniform electric field. The TOF method is widely used, especially in the case of the normal transport where the mobility μ and diffusivity D are constant and related by the Einstein’s relation $D/\mu = kT/e$. The case of the normal transport will be considered in present work. In the conventional TOF experiment technique for calculating mobility μ from the measured time of flight t_f, the effect of diffusion is not taken into account: $\mu = L/(t_f F_0)$, where L is the layer thickness. However, when the electric field or the layer thickness decreases, diffusion significantly distorts the TOF transient shape. This circumstance requires a revision of the conventional TOF technique applicability and an improvement of the TOF method in the calculation part for the correct determination of mobility, which will be discussed below. The TOF method has two mostly used experimental setups: TOF (surface generation of charge carriers) and TOF-2 (spatially-uniform generation of charge carriers). The TOF setup and its distortion by diffusion are analyzed and verified by the Monte Carlo simulation[1] from the point of view of a correct mathematical description of the physical experiment essence. The TOF-2 setup and its distortion by diffusion are considered below (see also Fig. 1).

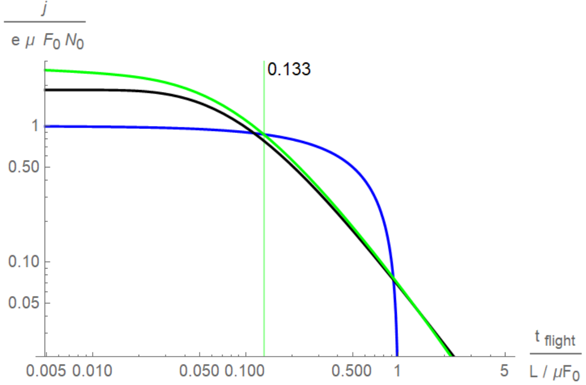

Fig. 1. TOF-2 transient (spatially-uniform generation of charge carriers) with $D/(\mu F_0 L) \approx 3.688$ (N_0 is the initial concentration of charge carriers). Blue color: only drift. Black color: only diffusion. Green color: both drift and diffusion. Vertical line shows the time of flight

Present work considers not only TOF-2 setup distortion by diffusion but theoretical generalization of both setups. In particular, numerically accurate analytic expressions for the ratio of the time of flight t_f to the normalizing value $L/(\mu F_0)$ are obtained and a method for determining mobility μ from TOF experiment data in thin layers of organic crystals is proposed, taking into account diffusion. Also, numerically precise limits of applicability of the conventional TOF technique have been generally formulated both for TOF and TOF-2 setups.

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Synthesis, Study of Structure-Property Relationships and Comparative Analysis of New Annelated Push-Pull Semiconductors Based on Indolo[3,2-B]Indole and Benzothieno[3,2-B]Benzothiophene

L.A. Poletavkina[1*], *I.V. Dyadischev*[1], *A.V. Bakirov*[1], *E.A. Svidchenko*[1], *N.O. Dubinets*[1], *Yu.N. Luponosov*[1]

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Organic semiconductor materials are actively developed and researched, which opens up broad prospects for the development of modern scientific and technological areas. Before synthesizing new compounds, it is extremely important to carefully design their structure, since it determines not only the conductive and electrochemical properties, but also the phase behavior, solubility and ability to certain types of crystal packing, which ultimately affects the electrical characteristics and the possibility of creating functional devices[1]. Of particular interest are structures combining electron-donor (D) and electron-acceptor (A) fragments (D-A). Such systems allow, by varying the strength and nature of the donor and acceptor components, to control molecular energy levels in a wide range, achieving the desired properties in target compounds[2]. Organic molecules built on the basis of condensed heteroaromatic fragments are of particular interest, since their rigid structure provides effective π-conjugation, high conductivity, oxidation stability and dense molecular packing[3].

In the work a number of semiconductor oligomers of D-A structure are synthesized, which are based on donor heteroaromatic fragments: known benzothieno[3,2-b]benzothiophene[4] and indole[3,2-b]indole. Keto- and dicyanovinyl fragments are used as acceptor groups, and the role of conjugated π-spacers linking D and A parts of the molecules is performed by benzene links. The schemes of synthesis of new semiconductor oligomers and the results of studies of their physicochemical properties will be shown: electrochemical, optical and thermal, phase behavior, analysis of the crystal structure including thermal PCA. Based on the presented data, the relationships between the structure and final properties of the obtained substances will be revealed, what effect the components and their replacement have on the physicochemical properties, a comparison of two donor blocks with each other, an assessment of the effect of sulfur and nitrogen heteroatoms. The identified relationships will allow us to draw conclusions about how to control and achieve the desired properties of organic semiconductors of this type. An assessment of the possibilities and prospects for using the obtained materials in organic electronics applications was also made.

The work was carried out with financial support from the Ministry of Science and Higher Education of the Russian Federation (contract No. 075-15-2024-532-2 within the framework of grant No. 075-15-2024-532).

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P-21

Optical Study of Non-Conjugated Polymers with Different Main Chain Nature for OLED Applications

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Both low-molecular-weight and high-molecular-weight compounds are used to improve the properties of organic light-emitting diodes (OLED). Despite the success of using small molecules, industrial production requires optimizing such properties as thermal and oxidative stability, service life, and adaptability. To solve these problems, the concept of non-conjugated polymers with pendant chromophores, analogues of small molecules, is proposed[1,2].

One of the widespread photosystems is the carbazole/triazine-1,3,5 donor-acceptor (DA) pair, which makes it possible to create a blue OLED[3,4,5,6]. A special feature of this molecular system is the presence of a thermally activated delayed fluorescence (TADF) mechanism, which allows fine-tuning of photovoltaic characteristics.

In this work, 9-N-phenylcarbazole and 2,4,6-trisphenyltriazine-1,3,5 were synthesized, which were selected as models for studying the optical properties of four polymers with different types of main chains – polystyrene and polysiloxane – and the DA ratio of fragments (Fig.1). The obtained models were characterized by NMR spectroscopy and HPLC. Comparative analysis has shown that effective TADF exists in the studied polymers.

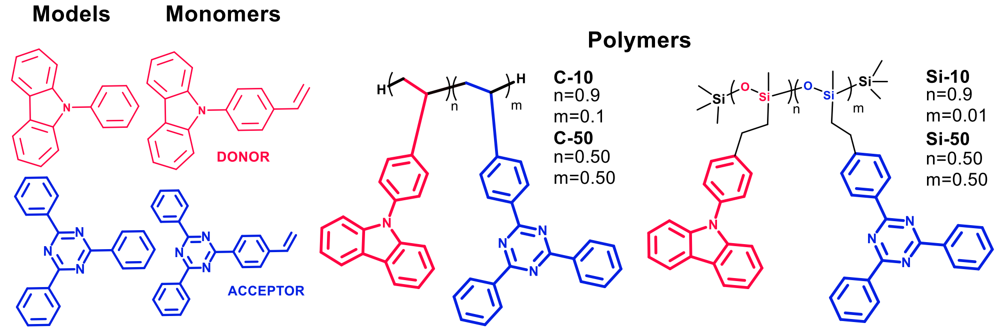

Fig. 1. Molecules which are used in optical study

This work was supported by FFSM (project FFSM-2024-0003).

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Polymer Materials for Use in Light-Emitting Diodes

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Polymer-based light-emitting diodes (PLEDs) offer advantages such as flexibility, lightweight design, and low production costs. However, their widespread use is limited due to material degradation under environmental factors. This study used a Fourier-transform spectrometer (Infralum FT-801) to analyze the degradation of polymer materials used in PLEDs.

Four polymers were examined: three emissive powders (F8BT, MEH-PPV, PFO) and one conductive liquid polymer (PEDOT:PSS). First, a reference spectrum (polyethylene or glycerol) was recorded, followed by spectra of the test materials. The results were compared with literature data to identify deviations indicating degradation.

Emissive polymers (F8BT, MEH-PPV, PFO): Spectra matched reference data, confirming their stability and suitability for use.[1]

Conductive polymer (PEDOT:PSS): Spectral deviations were observed—some peaks weakened while others intensified, indicating oxidation and material degradation.

The study showed that emissive polymers retain their properties and are suitable for PLED applications. However, the conductive polymer PEDOT:PSS requires regeneration or replacement due to degradation. To improve PLED stability, further research into degradation mechanisms and protective measures is needed.

Fig. 1. Experimentally captured spectrum PEDOT:PSS

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P-23

Terminal Groups Impact on The Properties of 2,1,3-Benzothiadiazole-Based Phenylene Derivatives

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Recently, there has been a significant interest in donor-acceptor systems for organic electronic applications. Researchers are actively working to enhance the properties of molecules by modifying individual components[1]. 2,1,3-Benzothiadiazole (BTD) is commonly utilized as an acceptor unit owing to its impressive optoelectronic characteristics and its ability to form efficient luminophores when paired with donor units[2]. The introduction of alkyl substituents makes possible to increase the solubility and lower the melting point of such compounds. Soluble fluorophores with a low melting point, a large Stokes shift, and a high quantum yield are commonly used in the production of plastic scintillators, in scintillating and spectroscopic optical fibers, large-scale detectors based on liquid scintillators designed to study cosmic rays and high-energy neutrinos.

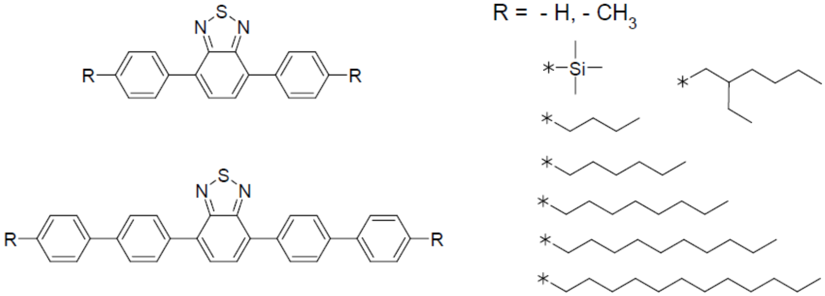

Fig. 1. Chemical structure of the obtained fluorophores

The purpose of this study is to investigate the relationship between the structure of novel linear organic luminophores and their photophysical, photochemical and thermodynamic properties. In this case, a series of symmetrical molecules comprised of a BTD core as the electron-withdrawing component and benzene moieties as donating units were synthesized via Suzuki cross-coupling reaction. Additionally, molecules with various terminal substitutions, such as trimethylsilyl derivatives, as well as derivatives with diverse alkyl chains, were synthesized in order to examine the influence of terminal groups on the properties of target molecules. The emission-luminescent properties of these derivatives, as well as their thermal characteristics through differential scanning calorimetry and thermogravimetric analysis, were studied to assess the impact of the terminal groups.

This work was supported by RSF № 22-13-00255-P.

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P-24

Synthesis and Physicochemical Properties of Thiophene-Containing Derivatives of 4,5-Diazafluorene

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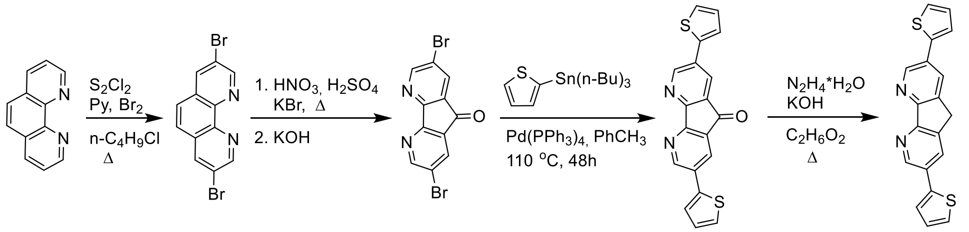
Linear conjugated small molecules and polymers are in high demand in organic optoelectronics. These materials are used in various devices such as OLEDs, sensors, solar cells, field-effect and light-emitting transistors. One particularly promising class of semiconductor and luminescent materials are fluorene derivatives, including oligofluorenes[1] and polyfluorenes.[2] However, 4,5-diazafluorene derivatives are much less studied and are presented only by limited examples, although due to their electronegative character and chelation ability, such compounds could be used to develop new functional materials.

In this work, 2,7-di(thiophen-2-yl)-9H-(4,5-diazafluorene)-9-one (TDAFO) and 2,7-di(thiophen-2-yl)-9H-4,5-diazafluorene (TDAF) (Fig. 1) were synthesized, their structures, physicochemical, electrochemical and optical properties were evaluated. The electropolymerization of TDAFO was demonstrated. Photoluminescence quantum yields of 73% and 13% were shown for TDAF and T-DAFO crystals. However, both materials demonstrated no semiconductor properties.



1 **2** (76%) **3** (45%) **TDAFO** (66%) **TDAF** (57%)

Fig. 1. Synthesis of 2,7-di(thiophen-2-yl)-9H-(4,5-diazafluorene)-9-one (TDAFO) and 2,7-di(thiophen-2-yl)-9H-4,5-diazafluorene (TDAF)

This work was supported by RSF (project № 23-73-10015).

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P-25

Centrosymmetric Donor-Acceptor TADF-Emitters for Single-Layer OLED Exhibiting Aggregation-Induced Emission

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Single-layer OLED architecture offers significant advantages over conventional multilayer design, primarily through reducing the number of organic compounds required for device fabrication. Recent studies demonstrate the efficiency metrics of single-layer devices containing a TADF emitter can not only match but even surpass those of their more prevalent predecessors[1]. The benefits of this approach has driven the emergence of studies performing high-throughput virtual screening of novel emissive materials for single-layer OLEDs.

Since ambipolar, trap-free and effective charge transport is prerequisite within single-layer concept, an emitter should have a broad recombination zone and a small dipole moment. Thus, taking into account a specific combination of donor-acceptor fragments, and molecular centrosymmetry, the most promising candidates were identified[2].

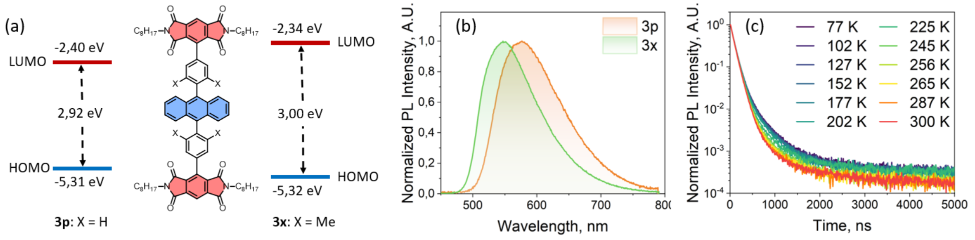

Fig. 1. (a) Experimentally identified energy levels of the frontier molecular orbitals, (b) promt photoluminescence of **3p** and **3x** in solid state, $\lambda_{ex} = 405$ nm, and (c) transient photoluminescence decay characteristics of **3x** in solid state at 77-300K, $\lambda_{ex} = 375$ nm

Here, we developed a synthetic route to donor 9,10-diarylanthracene cores connected to acceptor diimide fragments via phenylene or dimethylphenylene linkers. Photophysical analysis revealed both target compounds, **3p** and **3x**, exhibited weak red photoluminescence in solution ($\Phi_F < 0.2\%$) with broad emission maximum at 620 nm and 585 nm, respectively, which is attributed to twisted intramolecular charge transfer. A dramatic increase in quantum yields was observed in the solid state ($\Phi_F = 32–62\%$), which is consistent with aggregation-induced emission behavior. Compound **3x** was demonstrated to display TADF in thin films with $E_a = 119$ meV, which highlights its potential for single-layer OLED applications.

This work was supported by Ministry of Science and Higher Education of Russian Federation (project No. FSUS-2021-0014).

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Synthesis of Copolymers with Grafted Biotin-Containing BTBT Segments Based on Polysiloxane and Polystyrene

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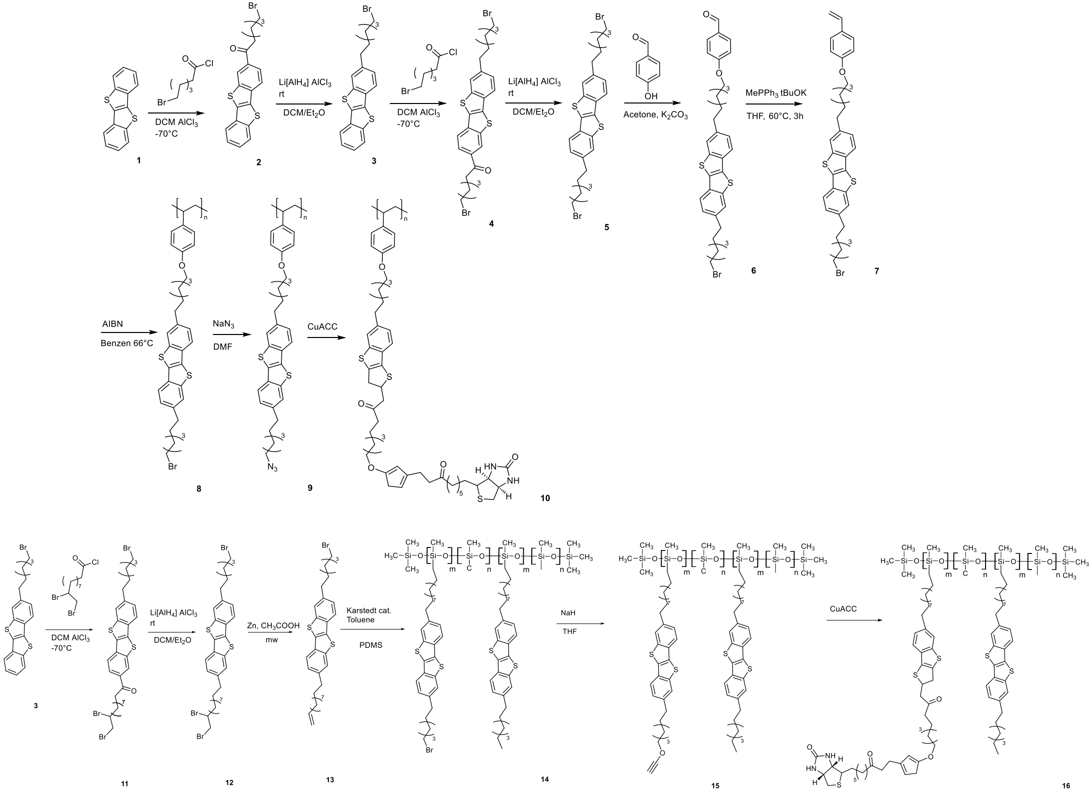
Among the various low-molecular-weight organic semiconductorsOSC structures, [1]benzothieno[3,2-b]benzothiophene (BTBT) stands out as a highly effective core for developing high-performance OFETs.

The functionalization of the surfaces of organic semiconductors or gate electrodes with biological receptors, by immobilizing molecules that are specific to target biomarkers enables selective analyte binding, which is essential for biosensing applications.

Currently, BTBT-based chemistry is undergoing extensive investigation, with a strong focus on structural modifications aimed at enhancing solubility, crystallinity, and stability. In this context, aliphatic fragments bearing reactive chloraldehyde groups are used to introduce alkyl chains selectively at the 2- and 7-positions of the BTBT core.[1,2]



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Functional and Non-Functional Oligomers Based on 4,4’-Bis(2,1,3-Benzothiadiazole)

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The interest in donor-acceptor molecules containing 2,1,3-benzothiadiazole fragments as an acceptor group is due to the unique optical and electrical properties of these molecules. Such polymers and oligomers are characterized by high temperature resistance, high absorption coefficients suitable for applications in organic photonics and electronics, values of the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO) as well as strong intermolecular interactions of pi-electronic systems. Therefore, the identification of the relationship between molecular structure and spectral, luminescent, thermal, and electrical properties is an urgent task for fundamental science as well as important for applied research on new oligomers containing 4,4’-bis(2,1,3-benzothiadiazole).

The main goal of this work is to develop and synthesize several new oligomers based on 4,4'-bis(2,1,3-benzothiadiazole), with a variety of donor substituents, and also to investigate the relationship between the chemical structure and properties of these systems. One of the main objectives was to develop an efficient method for producing 4-bromo-2,1,3-benzothiadiazole, a key intermediate, and to select the most suitable method for its purification.

The work was carried out with the support of the RSF (project № 22-13-00255-P).

Novel Chromophores, Incorporating 2,3-Diphenylthiophene Moieties

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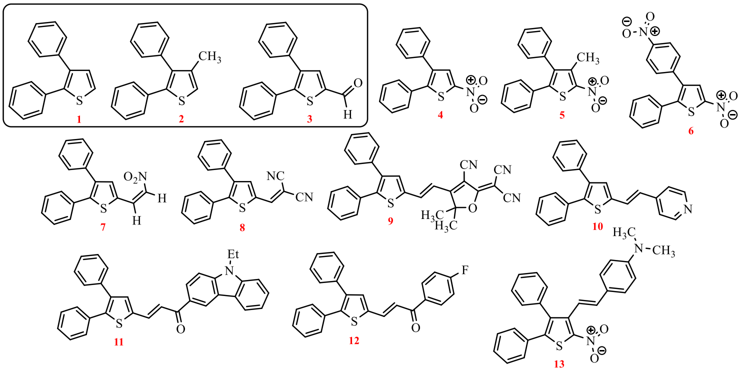
Analysis of the literature shows that such diaryl-substituted thiophenes as 2,3-diarylthiophenes (the so-called single-walled diarylthiophenes) are most often used in the field of organic electronics of all the diarylthiophenes. 2,3-Diphenylthiophene increasingly appears in the structure of π-conjugated small molecules used as components of materials for displays, organic electroluminescent devices, organic semiconductors, and light-emitting devices[1,2,3,4].



	λ^{em}_{max}, nm (Δ, nm)	E_{HOMO}/ E_{LUMO}, eV	E_g^{el}, eV
1	-	-5.24 -3.56	1.68
3	426 (86)	-5.21 -3.70	1.51
4	501 (123)	-5.29 -3.66	1.63
5	-	-5.20 -3.64	1.56
6	467 (112)	-5.23 -3.56	1.67
8	463 (56)	-5.59 -3.63	1.96
11	477 (82)	-5.73 -4.11	1.62
13	606 (102)	-5.00 -3.59	1.41

Fig. 1. Some examples of the thiophenes prepared, optical and electrochemical data

Using the substituted thiophenes **1-3** as the starting compounds, some functionalized thiophenes have been synthesized and studied (Fig.1). Each of them can be considered as a chromophore, in which the electron donating unit is a single-walled 2,3-diphenylthiophene moiety. Optical and electrochemical properties of the synthesized compounds have been investigated. Based on the data obtained, the optical bandgap width, the energies of the frontal orbitals, and the electrochemical bandgap width were determined. All the chromophores obtained can be classified as the narrow-band semiconductors.

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Optoelectronic Property Prediction and Generation of Multi-Resonance Thermally Activated Delayed Fluorescence Molecules Using Graph and Multimodal Neural Networks

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Thermally activated delayed fluorescence (TADF) materials with a twisted donor-acceptor structure suffer from strong vibronic coupling and structural relaxation, leading to a low oscillator strength (*f*) and broad emission spectra. In 2016, Hatakeyama et al. proposed a groundbreaking molecular design of TADF-emitters which is based on multiple resonance effect (MR, e.g. alternation of electron density in the molecule). Localization of boron and nitrogen atoms at *para*-positions into a six-membered ring led to effective short distant intramolecular charge-transfer, which in combination with fused polycyclic aromatic character significantly reduce vibrational motion of the emitter, and thus lead to narrowband emission.[1]

Development of novel functional materials—from conceptual molecular design through complex synthesis and extensive property characterization—remains a highly resource-intensive and time-consuming process. Modern computational approaches based on fine-tuned language models (LMs) offer promising new opportunities for the rapid discovery and generation of novel organic molecules with desired properties.[2]

We designed a range of MR-TADF emitters based on B,N-heteroarenes, which differ in the degree of structural tension due to steric repulsion between the central and peripheral parts of the emitter molecule. To significantly enhance computational efficiency and enable rapid molecular screening, we implemented and benchmarked two distinct machine-learning approaches: a GCN and a novel multimodal Transformer-based neural network. Based on GCN graph neural networks, an accelerated algorithm for predicting the energies of frontier orbitals, S_1 and T_1 has been developed. It is shown that the algorithm has a higher prediction accuracy in comparison with quantum chemical modeling based on DFT.

Importantly, multimodal Transformer model also enables accurate prediction of molecular electronic properties from given structures but also efficient at inverse molecular design—generating molecular structures conditioned on desired properties (bidirectional generation capability), a task not achievable with traditional GCN approaches. This research, therefore, offers a transformative workflow that substantially reduces experimental and computational resource on developing of novel MR-TADF OLED-emitters.

This work was supported by Russian Science Foundation and Ministry of Science and Higher Education of Russian Federation project No FSUS-2021-0014.

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P-30

Semiconductor Properties of Novel [1]Benzothieno[3,2-b][1]Benzothiophene Derivatives in OFETs Prepared by Solution Processing

Ya.O. Titova[1*], *L.L. Levkov*[1], *A.A. Trul*[1], *E.A. Sorokina*[1],
O.V. Borshchev[1], *S.A. Ponomarenko*[1,2]

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Organic semiconductors have a number of advantages, including flexibility, low trap density, high mobility of charge carriers and the ability to fine-tune properties through chemical modification. Derivatives of [1]benzothieno[3,2-b][1]benzothiophene (BTBT) are one of the most widely studied classes of compounds used as active elements in organic electronics, in particular in organic field effect transistors (OFETs). The high chemical and thermal stability of the BTBT fragment makes it possible to modify the structure by introducing conjugated substituents and solubilizing groups, which promotes the self-organization of semiconductor molecules into crystal lattices.

In this work semiconductor properties of three novel organic semiconductors – 3, 4 and 5-substituted isomers of dioctyl derivatives 2,7-dithienyl-BTBT (3-C8-T-BTBT, 4-C8-T-BTBT or 5-C8-T-BTBT) were investigated and compared with the properties of 2,7-dioctyl-BTBT (C8-BTBT) in OFETs with different architectures – top and bottom contacts (Fig. 1). The devices were prepared by three different solution-processing methods: drop casting, doctor blade and spin-coating. It was shown that C8-BTBT and 5-C8-T-BTBT exhibit the best semiconductor properties among the BTBT derivatives investigated – their charge carrier mobility reaches 1.7 and 1.1 cm^2/Bc, respectively.[1]

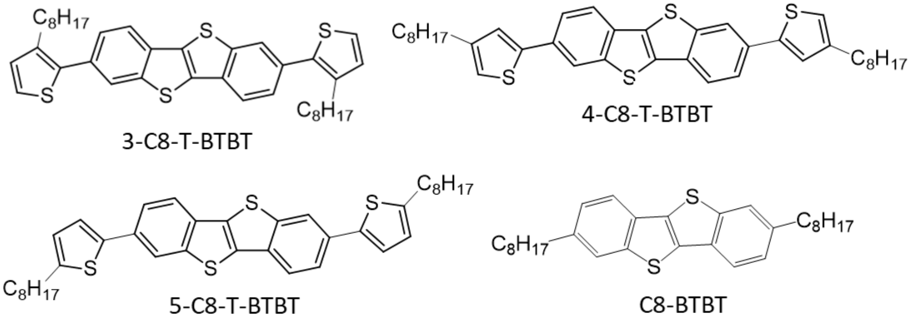

Fig. 1. The structure of three isomers of dioctyl derivatives of 2,7-dithienyl[1]benzothieno[3,2-b][1]benzothiophene

The work was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (contract No. D24-0493 within the framework of grant No. 075-15-2024-560).

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P-31

Organic Light-Emitting Diodes Based on Thienyl-Containing Derivative of Tris(2,4,6-Trichlorophenyl)Methyl Radical

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Organic light-emitting diodes (OLEDs) typically use closed-shell materials in which electrons are paired, and molecular orbitals are filled up to the highest occupied molecular orbital (HOMO) according to the Aufbau principle. Upon applied voltage, electrons and holes are injected into the emission layer, forming 25% singlet and 75% triplet states, according to spin statistics. Therefore, the well-known problem of spin statistics dictates that the maximum electroluminescence (EL) efficiency is limited to 25%, since only singlet excitons are spin-allowed for radiative decay, while most triplet excitons dissipate energy as heat. To overcome this problem, triplet states are involved in the radiation process by the incorporation of transition metals to promote phosphorescence via heavy metal-enhanced spin-orbit coupling and indirectly by thermally activated delayed fluorescence or triplet-triplet annihilation. Another approach to control emissive states in OLEDs has emerged with stable organic radicals, mainly based on tris(2,4,6-trichlorophenyl)methyl (TTM).[1,2] In such materials both the ground and first excited states have a doublet-spin character and that emission is totally spin allowed. The main advantages of OLEDs based on luminescent radicals are their low synthesis cost, short fluorescence lifetime, and efficient pure deep red and near infrared emission.

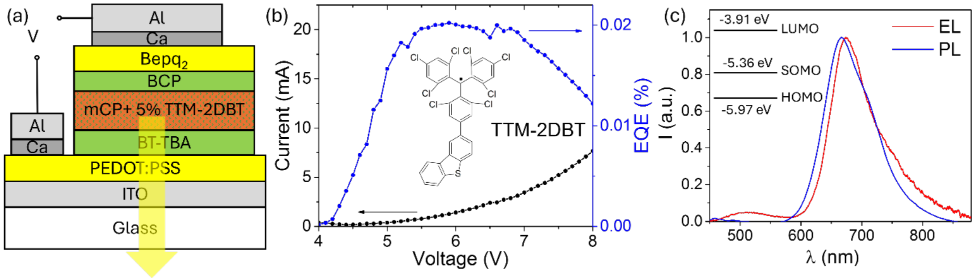

Fig. 1. Scheme of TTM-2DBT-based OLED structure (a), its current-voltage characteristics and external quantum efficiency (EQE), inset shows TTM-2DBT molecular structure (b), and its EL spectra compared to PL spectra of TTM-2DBT solid solution in PMMA film, inset shows energy levels of TTM-2DBT molecular orbitals (c)

In this work we propose OLEDs based on novel TTM-based radical derivative, TTM-2DBT. Its photoluminescence (PL) provides pure deep red light with CIE coordinates x=0.67, y=0.28. EL spectra of fabricated TTM-2DBT-based OLEDs have peak at 675 nm and are almost coincide with radical PL spectra except for slight red shift. However, the external quantum efficiency (EQE) of OLED EL is rather low (about 0.02%), most likely because of the not optimal matrix semiconducting material, hole/electron transport layers and electrodes. It is expected that the selection of proper organic semiconductors and electrode materials in OLED with novel radical luminophore TTM-2DBT will lead to enhancement of EQE by orders of magnitude, exceeding that of other LEDs with deep red emission.

This work was supported by RSF (project № 24-49-02038).

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Grafted Polymers with Benzothieno[3,2-B]Benzothiophene (BTBT) Moieties as Side Groups: Prospects for High-Performance Organic Semiconductors

E.A. Zaborin[1*], *O.V. Borshchev*[1], *P.A. Shaposhnik*[1], *Ya.O. Titova*[1], *V.V. Gorodov*[1],
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The transition from small molecules to polymeric materials is a critical step in advancing large-area ink-jet printing technologies, which are increasingly important for flexible, lightweight, and cost-effective electronic devices. Polymers offer numerous advantages over small molecules in printing applications, including enhanced processability, improved environmental stability, and the potential for scalable, low-cost manufacturing processes. These benefits enable the production of high-quality, uniform thin films over large surfaces, essential for commercial applications.[1]

This study reports the synthesis and comprehensive characterization of novel comb-shaped polymers featuring benzothieno[3,2-b]benzothiophene (BTBT) fragments as side substituents. The incorporation of BTBT units imparts unique electronic properties to these polymers, such as increased conjugation length and improved charge transport capabilities. These materials demonstrate promising potential for use in various organic electronic devices, including organic field-effect transistors (OFETs), organic solar cells (OSCs), and other optoelectronic applications.

The research is particularly significant due to its innovative approach—designing and synthesizing comb-shaped architectures with BTBT side groups—which has not been extensively explored in the literature.[2,3] The structural design aims to enhance molecular ordering and π-π stacking interactions, thereby improving charge mobility and device performance.[4] The study investigates the structural features, electronic properties, and ability of these polymers to form ordered morphologies on substrates.

Findings from this work lay a foundation for further development of advanced organic electronic materials. They open pathways toward optimizing polymer structures for better device efficiency and stability, ultimately contributing to the evolution of flexible electronics, large-area printed devices, and next-generation optoelectronic systems.

The work was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (contract No. D24-0493 within the framework of grant No. 075-15-2024-560).

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Synthesis and Properties of П-Conjugated Molecular Liquids with Trihexylsilyl Terminal Substituents

I.V. Dyadishchev[1], *D.O. Balakirev*[1], *E.A. Svidchenko*[1], *N.M. Surin*[1], *S.A. Ponomarenko*[1], *Yu. N. Luponosov*[1]

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Functional molecular liquids are relatively new and class of materials, which have high processability owing to their fluidic nature and efficient fluorescence in pristine state[1]. They are already finding application in various fields of optoelectronics. However, the structure-property relationships of such compounds remain poorly understood. In addition, they exhibit luminescence in a limited short-wavelength region of the spectrum. Most of the molecules with long wavelength or NIR absorption and luminescence have a rigid planar structure due to their large π-conjugation.

In the course of this work, the series of novel benzothiadiazole-based molecular liquids, emitting light in various ranges of the visible spectrum, were synthesized. To liquefy these compounds the trihexylsilyl terminal substituent as most effective solubilizing group[2]. The high purity and specified structure of all the compounds obtained was proved by a complex of modern research methods. The influence of the nature, length, branching and type of π-conjugated core on the optical properties, rheology, phase behavior and thermal stability of luminophores has been studied. Some of the obtained oligomers were tested as scintillation detectors[3]. Due to the high concentration of active phosphor fragments per unit volume in such materials, which cannot be achieved by preparing a simple solution based on them, and the relatively high fluorescence quantum yield in the block (up to 75%), effective scintillators based on these oligomers were created.

This work was supported by the Russian Ministry of Science and Education (project no. FFSM-2024-0003).

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Electrolyte-Gated Organic Field-Effect Transistor as a Perspective Platform for Detecting Metals in Aqueous Solutions

B.S. Kuleshov[1*], *E.Yu. Poimanova*[1], *D.A. Skvortsov*[1], *E.V. Agina*[1,2], *S.A. Ponomarenko*[1,3]

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[2] Lomonosov Moscow State University, Department of Fundamental Physical and Chemical Engineering
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Electrolyte-gated organic field-effect transistors (EGOFETs) (fig. 1) have garnered significant interest in biosensing applications due to their unique properties. These devices are particularly well-suited for analyzing liquid samples, as the dielectric layer that typically separates the gate electrode and organic semiconductor in other types of field-effect transistors is replaced by an electrolyte solution. This allows for greater flexibility and compatibility with liquid samples, making EGOFETs a promising technology for biosensing. Another key advantage of EGOFETs is their extremely high capacitances, which can reach up to several hundred μF cm^{-2} when using an electrolyte[1]. The creation of a sensor capable of quickly and selectively detect metal ions in biological fluids is a promising task for the development of a simple and mobile device capable of monitoring a person's condition outside a medical institution. The proposed approach to creating a receptor layer of the device provides the possibility of creating a universal platform for further recognition of alkali metal ions through the use of structures containing crown ether groups binding to a previously developed universal support layer.[2]

In the course of this work, various materials, mainly crown esters and aptamers, were used to manufacture receptor layer of EGOFET devices in order to detect ions of various metals. The results of the Voltametric characteristics obtained during the measurement were used to determine the dependence of the response of the obtained devices on the concentration of metal ions and describe the obtained patterns.

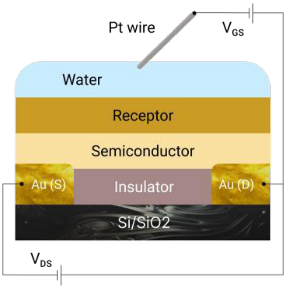

Fig. 1. Principial scheme of the proposed EGOFET device

The behavior of EGOFET under the influence of various concentrations of various metal ions was studied. A morphological analysis of the surfaces of devices obtained by applying receptor layers capable of selectively binding ions of various metals has been carried out. The influence of interfering ion and ionic strength factors on the measurement results is shown. It is planned to create a full-fledged multi-sensor device capable of detecting the concentration of ions of various metals in a solution in real time.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project № FFSM-2025-0001).

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[1] Piro, B., Mattana, G., & Reisberg, S. *Biosensors*. 2018, **8**(3), 65.

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СКОРОХОД – УНИВЕРСАЛЬНАЯ ПЛАТФОРМА ДЛЯ УНИКАЛЬНЫХ РЕШЕНИЙ

- ✓ **ФОТОМЕТРИЧЕСКИЕ ДЕТЕКТОРЫ** (СФД И ДМД) С ДВОЙНЫМ ТЕМПЕРАТУРНЫМ КОНТРОЛЕМ. ДРЕЙФ: 3×10^{-4} Е.О.П./Ч
- ✓ **АВТОДОЗАТОР** ПРЯМОГО ДОЗИРОВАНИЯ ПРОБЫ ИЗ ИГЛЫ «SPLIT-LOOP" (ЕДИНСТВЕННЫЙ В РФ)
- ✓ **НАСОСЫ** КОРОТКОХОДОВЫЕ БЕЗПУЛЬСАЦИОННЫЕ

SEVKO

ПРОИЗВОДИМ, А НЕ СОБИРАЕМ

- СОБСТВЕННАЯ РАЗРАБОТКА И ПРОИЗВОДСТВО ПОЛНОГО ЦИКЛА
- ГОТОВЫЕ НАБОРЫ ДЛЯ ЕЖЕГОДНОГО ТО
- УНИКАЛЬНЫЕ ДЛЯ РОССИЙСКОГО РЫНКА ТЕХНИЧЕСКИЕ РЕШЕНИЯ
- 2 ГОДА ГАРАНТИИ
- НЕЗАВИСИМОСТЬ ОТ ДЕФИЦИТНЫХ ЗАПАДНЫХ КОМПОНЕНТОВ
- ЗАМЕНА ВСЕХ РАСХОДНЫХ МАТЕРИАЛОВ СИЛАМИ ПОЛЬЗОВАТЕЛЯ
- НИЗКАЯ СТОИМОСТЬ ВЛАДЕНИЯ ПРИБОРОМ
- ВОЗМОЖНОСТЬ КАСТОМИЗАЦИИ

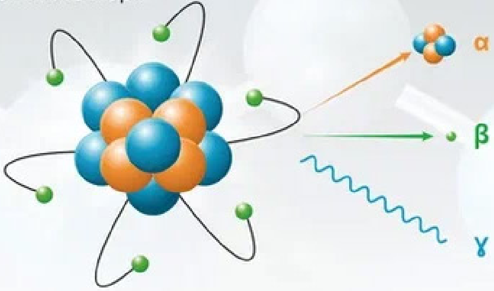
ЛУЧШЕЕ ДЛЯ СВОИХ

SKOROHOD

- ✓ **СТОЙКОСТЬ** КО ВСЕМ ОРГАНИЧЕСКИМ РАСТВОРИТЕЛЯМ, PH = 1-14
- ✓ **КОМПАКТНОСТЬ** (НА 35-50% МЕНЬШЕ МОНОБЛОКОВ ЗАПАДНОГО ПРОИЗВОДСТВА)
- ✓ **СООТВЕТСТВИЕ ПО** 21 CFR PART 11. ПРЯМОЕ **УПРАВЛЕНИЕ ВСЕМИ МОДУЛЯМИ** ЭКОСИСТЕМЫ «СКОРОХОД»

Уникальное отечественное решение для ВЭЖХ радиофармпрепаратов: хроматограф "Скороход" с γ-радиометрическим детектором

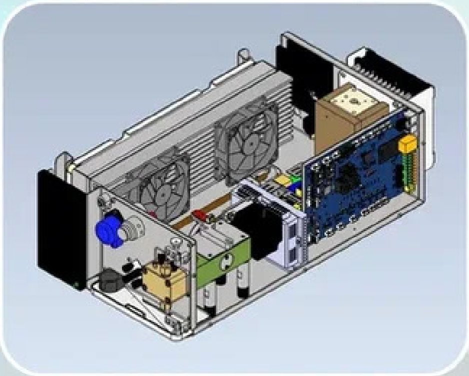
- Регистрация в реальном времени γ-спектра радионуколида с возможностью построения 3D-хроматограммы.
- Настраиваемая геометрия детектора для работы в аналитическом и препаративном режимах.
- Быстрая смена детекторов γ- и β-излучения. Детектор для α-излучающих радионкулидов.
- Автодозатор прямого дозирования (split-loop) для ввода самых малых объемов без перерасхода пробы или полуавтоматический ручной инжектор.



Модуль постколоночной дериватизации из серии ВЭЖХ "Скороход". Готовые решения, проверенные временем

Анализ аминокислот

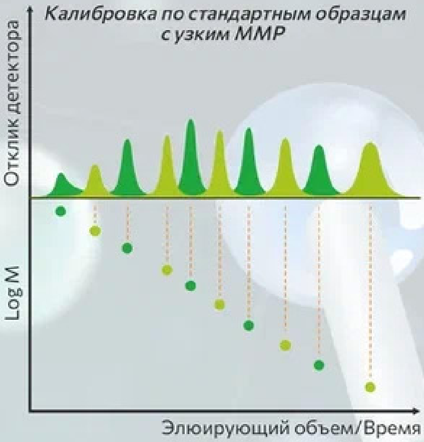
- Оригинальная разработка на основе отечественной компонентной базы.
- Единственный модуль постколоночной дериватизации в РФ: более 10 лет успешной работы с хроматографами разных марок.
- Инертное исполнение ВЭЖХ-системы.
- Лоток для бутылей с системой подачи инертного газа.
- Катионообменные колонки собственного производства.
- Набор реагентов для определения аминокислот в комплекте.
- Демонстрация методики на вашей площадке.

Альтернативные применения постколоночной дериватизации

- Биогенные амины.
- Монезин, наразин и салиномицин.
- Мадурамицин аммония, семдурамицин натрия, гидрат гадодиамида.
- Редуцирующие и фосфорилированные редуцирующие сахара.
- Анионы переходных и тяжелых металлов.
- Водорастворимые витамины B1, B2, B6 (ГОСТ 32903-2014).
- Афлатоксин B1 (ГОСТ 32251-2013, EH-12955) и сумма афлатоксинов B1, B2, G1 и G2 (EH-12955).

ХРОМАТОГРАФ «СКОРОХОД» ДЛЯ АНАЛИЗА ПОЛИМЕРОВ МЕТОДОМ ГПХ



- Единое ПО Мультихром для управления прибором и обсчета данных ГПХ.
- Непревзойденные повторяемость (0,06 % ОСКО) и точность (± 0,15 %) потока подвижной фазы, а также стабильность поддержания температуры (± 0,1 °С) гарантируют отсутствие ошибок при определении ММ полимеров.
- Стойкость к ТГФ, ДМФА, ДМСО, ДМАА, ГФИП, хлорированным растворителям.
- Вместительный термостат для работы с каскадами колонок.
- Широкий температурный диапазон (до 99 °С).
- Плавное увеличение скорости потока подвижной фазы во избежание повреждения частиц полимерного геля.
- Разнообразие концентрационных детекторов (РФД, СФД, ДМД, СРД).
- Инертное исполнение для работы с биомолекулами.

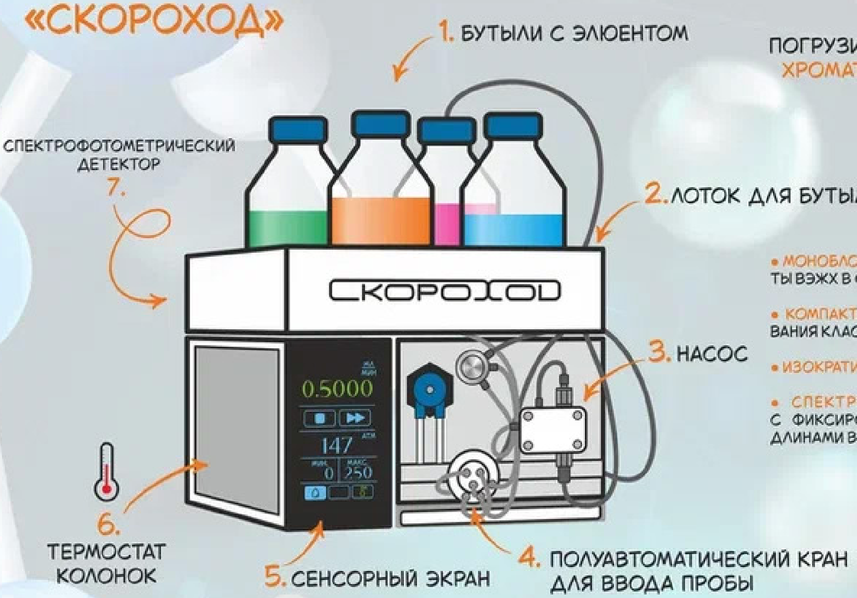
Частица полимерного геля
(поперечное сечение)

УЧЕБНЫЕ ХРОМАТОГРАФЫ «СКОРОХОД»

УЧЕБНЫЙ ВЭЖХ «СКОРОХОД»

СОВЕРШАЙ ОТКРЫТИЯ
ВМЕСТЕ СО СКОРОХОДОМ!

ПОГРУЗИСЬ В УВЛЕКАТЕЛЬНЫЙ МИР
ХРОМАТОГРАФИИ ВМЕСТЕ С НАМИ!



- МОНОБЛОЧНОЕ ИСПОЛНЕНИЕ - ВСЕ КОМПОНЕНТЫ ВЭЖХ В ОДНОМ КОРПУСЕ
- КОМПАКТНОСТЬ - ПОДХОДИТ ДЛЯ ОБОРУДОВАНИЯ КЛАССОВ И АУДИТОРИЙ
- ИЗОКРАТИЧЕСКИЙ ИЛИ ГРАДИЕНТНЫЙ РЕЖИМЫ
- СПЕКТРОФОТОМЕТРИЧЕСКИЙ ДЕТЕКТОР С ФИКСИРОВАННЫМИ ИЛИ ПЕРЕКЛЮЧАЕМЫМИ ДЛИНАМИ ВОЛН

ПРЕПАРАТИВНЫЕ И ПОЛУПРЕПАРАТИВНЫЕ ХРОМАТОГРАФЫ «СКОРОХОД»

- Насосы производительностью 150 мл/мин, 40 мл/мин и 10 мл/мин.
- Автоматический коллектор фракций, гибко конфигурируемый под любые приемные сосуды, или автоматические краны для сбора фракций.
- Держатели аналитических, препаративных и полупрепаративных колонок.
- Любые детекторы: СФД, ДМД, РФД, ФЛД, СРД с ячейками, соответствующими масштабу разделения.
- Автоматический сбор фракций по программируемым сигналам детектора при помощи ПО Мультихром.
- Инертное исполнение для работы с биомолекулами.
- Расчет и масштабирование системы из аналитической.

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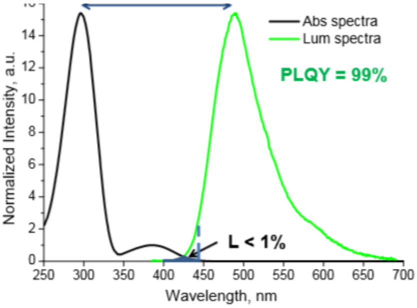
LumInnoTech

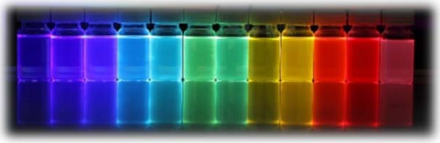
The main goal of LumInnoTech is research, development and commercialization of Nanostructured Organosilicon Luminophores (NOLs) with unique optical properties combining those of organic luminophores and inorganic quantum dots.

Key advantages of NOLs:

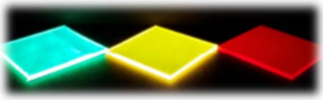
- High luminescence quantum yield: up to 99%
- High molar extinction coefficient: up to 300 000
- Large pseudo Stokes shift: up to 250 – 300 nm
- The possibility of controlling a wavelength of the light emission in a wide range
- Good solution processability
- High stability



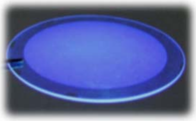
- ➢ **A library of NOLs, emitting at the desired wavelengths in the range from 390 to 650 nm.**

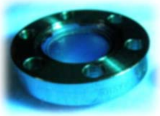


- ➢ **Wavelength shifting plates for pure CsI crystals**

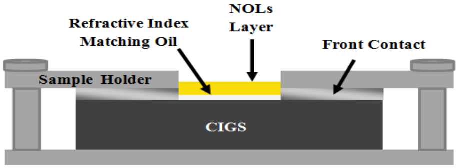


- ➢ **VUV wavelength shifters for improving photon detection efficiency of noble gas detectors**

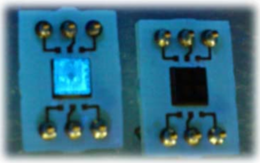




- ➢ **Luminescent Down Shifting Materials for CIGS Photovoltaics**



- ➢ **Effective Spectral Shifters for Silicon Photomultipliers**



- ➢ **New generation of highly efficient and fast plastic and organosilicon scintillators**

- ➢ **Various NOLs are available from 100 mg to 100 g quantity**

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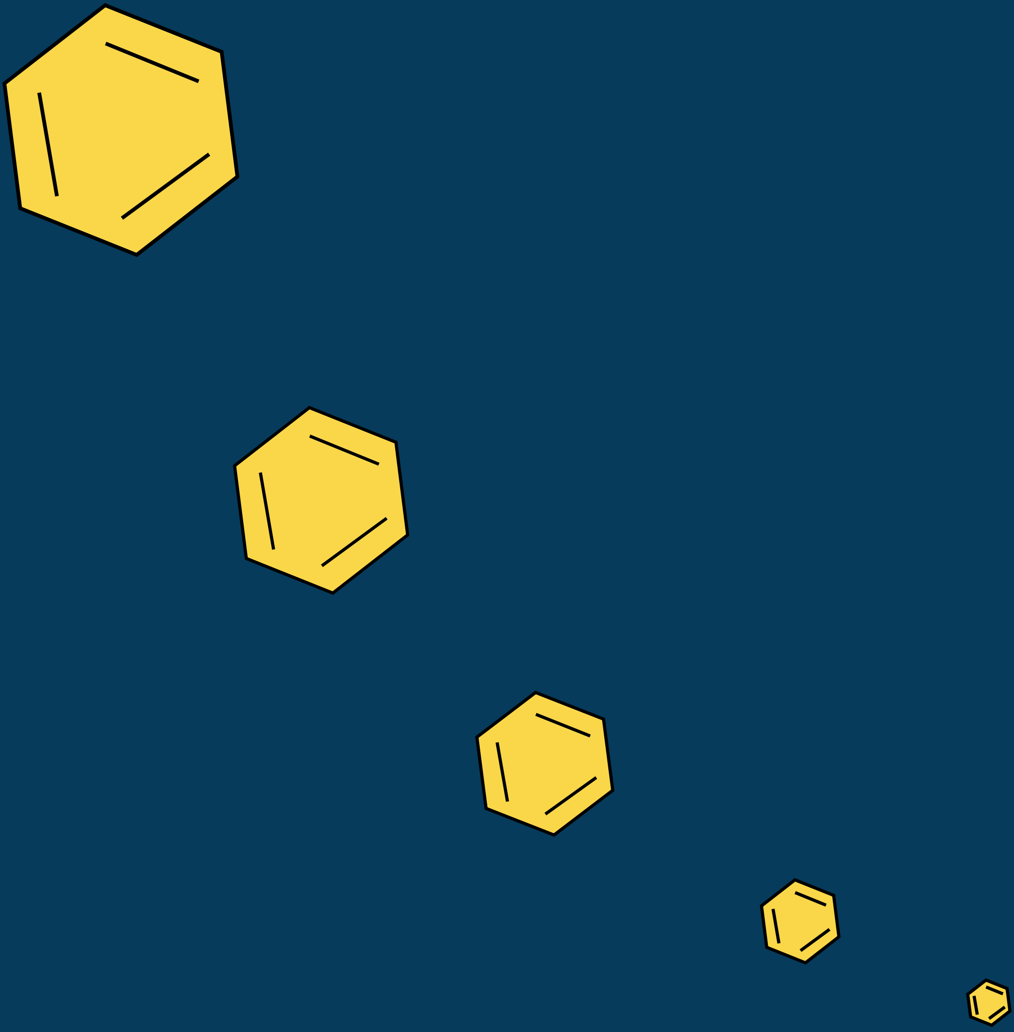
117393 Moscow, 70 Profsoyuznaya st., b. 1, of. 710. Tel.: +7 (495) 332 58 97, Fax: +7 (495) 335 90 00
LumInnoTech@gmail.com http://www.luminnotech.com

RSF Russian Science Foundation

LumInnoTech



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