



12th International Fall School on Organic Electronics

Book of Abstracts



September 13-17, 2026

Moscow, Russia

ISPM RAS

<https://ifsoe.ru/>

12th INTERNATIONAL FALL SCHOOL ON ORGANIC ELECTRONICS – 2026 (IFSOE-2026)

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)

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 12th International Fall School on Organic Electronics – 2026 Time Schedule Moscow, Russia (GMT+3)

Time	Sunday September, 13	Monday September, 14	Tuesday September, 15	Wednesday September, 16	Thursday September, 17
10:00	10:00 - 13:00 Registration at ISPM RAS	School Opening	Pavel Troshin	Dmitry Paraschuk	Georgy Pakhomov
		Valentine Ananikov	Huiqiong Zhou	Dmitriy Ionov	Dmitrii Ivanov
11:00		Egor Verbitskiy	Mahmoud Zendedel	Dmitry Maslennikov	Sergey Ponomarenko
		Aleksandr Yakimansky	Coffee-break	Coffee-break	
12:00		Coffee-break			Carlos Cesar Bof Bufon
	Ilya Taydakov	Elena Poimanova	Nikita Dubinets	Farewell buffet	
13:00	Maxim Kazantsev	Lunch	Lunch		
	Lunch				
14:00	Raul David Rodriguez				
15:00	Oral talks 1	Olga Fedorova	Oleg Kharlanov		
		Oral talks 3	Oral talks 5		
16:00	Coffee-break + Poster session 1	Coffee-break + Poster session 2	Coffee-break		
17:00	Oral talks 2		Oral talks 6		
18:00		Oral talks 4			
19:00	Welcome party				

Sunday, September 13

10:00 – 13:00	Registration at ISPM RAS.
15:00 – 16:30	Excursion to the Moscow Kremlin

Monday, September 14

10:00 – 10:15	School Opening
	Chair: Maxim Kazantsev
10:15 – 11:00	T-1. Valentine Ananikov. Mechanisms of Catalytic Reactions in Organic Synthesis: How to Discover or Improve The Catalyst?
11:00 – 11:30	I-1. Egor Verbitskiy. 1,4-Diazatriphenylene and its Hetero-Fused Analogues: Synthesis and Applications
11:30 – 12:00	I-2. Aleksandr Yakimansky. Functionalized Polyfluorenes for Optoelectronics and Medicine
12:00 – 12:30	Coffee-break
	Chair: Aleksandr Yakimansky
12:30 – 13:15	T-2. Ilya Taydakov. Luminescent Materials Based on Lanthanide Coordination Compounds - Synthesis, Energy Transfer and Prospects for Practical Applications
13:15 – 13:45	I-3. Maxim Kazantsev. Diazafluorenes for Organic Optoelectronics and Sensorics
13:45 – 15:00	Lunch time
	Chair: Egor Verbitskiy
15:00 – 15:30	I-4. Raul David Rodriguez. Towards Elastic Electronics: Light-Driven Fabrication of Stretchable Nanocomposites
15:30 – 15:45	O-1. Anna Lipovka. Advanced Nanoscale Surface Analysis of Materials for Flexible Electronics and Sensors
15:45 – 16:00	O-2. Aleksandra Paderina. Pt(II) Complexes with Alkynylphosphine Oxide Ligands: Variety of Luminescent Properties in Polymeric Films
16:00 – 17:30	Coffee-break + Poster session 1 (P1 – P 15)
	Chair: Maxim Kazantsev
17:30 – 17:45	O-3. Tatiana Moshkina. D- π -A Structures Based on [1,2,4]triazolo[c]quinazolines: Multifunctional Fluorescent Molecules
17:45 – 18:00	O-4. Irina Gudkova. Synthesis of new comb-shaped polymers containing 2-undecyl-7-octyl-[1]benzothieno[3,2-b]benzothiophene moieties
18:00 – 18:15	O-5. Evgeniy Zaborin. Synthesis and Properties of Novel Promising Semiconducting Polymers for Organic Electronics
18:15 – 18:30	O-6. Lev Levkov. Conjugated Polymers Based on Alkylthiophene-Substituted Derivatives of Benzothieno[3,2-B][1]Benzothiophene
18:30 – 20:00	Welcome party

Tuesday, September 15

	Chair: Dmitry Paraschuk
10:00 – 10:45	T-3. Pavel Troshin. Organic Semiconductors for Space Applications: Modelling Intrinsic Photostability and Radiation Resilience Based on Structure Descriptors
10:45 – 11:15	I-5. Huiqiong Zhou. Interface Engineering in Organic and Perovskite Solar Cells
11:15 – 11:45	I-6. Mahmoud Zendejdel. Recent Achievements in The Development and Scaling of Perovskite Modules
11:45 – 12:15	Coffee-break
	Chair: Pavel Troshin
12:15 – 13:00	T-4. Carlos Cesar Bof Bufon. Vertical Organic Field-Effect Transistors: Fundamentals and Current Trends
13:00 – 13:30	I-7. Elena Poimanova. Biosensors Based on Organic Field-Effect Transistors
13:30 – 14:30	Lunch time
	Chair: Carlos Cesar Bof Bufon
14:30 – 15:15	I-8. Olga Fedorova. Photosensitive Organic-Inorganic Hybrid Materials for Gas Sensor Applications
15:15 – 15:30	O-7. Polina Shaposhnik. Novel polymers with BTBT-Containing Side Chains as Semiconducting Materials for OFETs
15:30 – 15:45	O-8. Askold Trul. Sensory Response Peculiarities of Organic Field-Effect Transistors
15:45 – 16:00	O-9. Pralay Chanda. Modulation of Trap Density for Low Voltage Operation in Solution Processed Organic Field Effect Transistor
16:00 – 16:15	O-10. Debajyoti Jana. CMC Dielectric-Based Organic Field-Effect Transistors for Low operational voltage, Flexible and Mimicking Biological Synapse
16:15 – 17:45	Coffee-break + Poster session 2 (P16– P 30)
	Chair: Huiqiong Zhou
17:45 – 18:00	O-11. Leonid Kulik. Direct Optical Generation of Interfacial Charge-Transfer States in Organic Donor/Acceptor Blends: What Is the Difference from Exciton-Mediated Generation?
18:00 – 18:15	O-12. Lyubov Frolova. Suppression of Light- and Radiation-Induced Halide Phase Segregation in CsPbI ₂ Br through Compositional Engineering
18:15– 18:30	O-13. Ekaterina Ilicheva. Optimization of slot-die printing technology of self-assembling monolayers on NiOx surface for perovskite solar cells
18:30– 18:45	O-14. Polina Sukhorukova. Development of Materials with an Anchor Group for Defects Passivation as Interfacial Layers in Perovskite Solar Cells
18:45 – 19:00	O-15. Nikita Emelianov. Identifying Stable Perovskite Absorbers and Charge Transport Layers Under Electric Field Stress

Wednesday, September 16	
	Chair: Alexander Romanov
10:00 – 10:45	T-5. Dmitry Paraschuk. How does OLED work?
10:45 – 11:15	I-9. Dmitriy Ionov. Molecular Singlet and Triplet States: Extracting Maximum Information from Photophysical Experiment
11:15 – 11:45	I-10. Dmitry Maslennikov. Time-Resolved Spectroscopy For New Optoelectronic Materials Discovery
11:45 – 12:15	Coffee-break
	Chair: Oleg Kharlanov
12:15 – 13:00	T-6. Alexander Romanov. Advances in metal-containing luminophores: thermally activated delayed fluorescence (TADF)
13:00 – 13:30	I-11. Nikita Dubinets. Design and multiscale modelling of new effective TADF-luminophores
13:30 – 14:30	Lunch time
	Chair: Dmitriy Ionov
14:30 – 15:15	T-7. Oleg Kharlanov. Charge transport collapse in organic semiconductors: Competing views and frameworks
15:15 – 15:30	O-16. Andrey Sosorev. Electron-vibrational coupling in boron-free multiple resonance fluorophores
15:30 – 15:45	O-17. Vasiliy Trukhanov. Blue Organic Light-Emitting Diodes Based on Novel Phenoxazine-Substituted Multiple Resonant Luminophore with Thermally Activated Delayed Fluorescence
15:45 – 16:00	O-18. Evgeny Mostovich. Rational Design of Sterically Twisted D- π -A- π -D Emitters for Single-Layer OLEDs
16:00 – 16:15	O-19. Darya Tarakanovskaya. Topological Analysis of Multi-Resonance Thermally Activated Delayed Fluorescence Materials Based on B,N-Heteroarenes for Krisc And Emission Bandwidth Prediction
16:15 – 16:45	Coffee-break
	Chair: Nikita Dubinets
16:45 – 17:00	O-20. Vladimir Nikitenko. Universal Analytical Approach for The Transport Energy and Mobility in Disordered Organic Semiconductors
17:00 – 17:15	O-21. Anna Saunina. Analytic Description of Charge Carrier Mobility in Materials with Correlated Disorder Based on Modified Effective Temperature Concept
17:15 – 17:30	O-22. Sergey Novikov. Bimolecular Charge Carrier Recombination in Amorphous Semiconductors Having Spatially Correlated Exponential Density of States
17:30 – 17:45	O-23. Igor Koskin. Fine-Tuning Directional Message Passing Neural Networks: Predicting Properties of Conjugated Organic Polymers with High Accuracy
17:45 – 18:00	O-24. Daniil Litvinenko. Monte Carlo Modelling of Geminate Pair Separation Probability in Disordered Organic Semiconductors

Thursday, September 17	
	Chair: Dmitry Paraschuk
10:00 – 10:45	T-8. Georgy Pakhomov. SIMS analysis of multilayer organic/inorganic structures
10:45 – 11:15	I-12. Dmitrii Ivanov. Modern In Situ Methods for Monitoring Supramolecular Structure Formation in Organic Semiconductors
11:15 – 12:00	T-9. Sergey Ponomarenko. Standards and guidelines for good practice in organic electronics: where do they come from and why do we need them?
12:00 – 12:30	School Closing
12:30 – 14:00	Farewell buffet

Poster session 1

Monday, September 14, 16:00

Abramov Pavel	P1	Copper Binding, Tautomeric Equilibrium, and Thermal Dehydration in Eumelanins
Abramova Evgeniya	P2	2,2'-bipyridines Functionalized with Diphenylphosphoryl Groups for Emitters Based on Transition Metal Complexes
Baranov Denis	P3	Bis(tetracyanoselenophenoanthraquinodimethane) as Electron Acceptor for Organic Solar Cells and Photomultiplication-Type Organic Photodetectors
Demianenko Alena	P4	Tuning of Synaptic Properties by Ionogel Composition in Biocompatible Electrolyte-Gated Organic Transistors for Neuromorphic Applications
Dorofeev Dmitri	P5	The Role of Ionic Migration and Cluster Formation in the Thermal Stability of CsFAPbI ₃ Perovskite Solar Cells
Dyadishchev Ivan	P6	Synthesis and Properties of Functional Fluorescent Molecular Liquids with Trihexylsilyl Terminal Substituents
Elovsky Roman	P7	Design and Photophysical Investigation of Highly Efficient Pyrene-Substituted Acridone Blue Emitters for OLED Applications
Fatykhov Ramil	P8	One-Pot Synthesis and Photophysical Properties of 4-Carboranylcoumarin Fluorophores
Filipenkov Dmitrii	P9	Impact of Layers Thickness Proportion on the Charge Carrier Recombination Profile in Organic Light Emitting Diodes
Gaikov Dmitri	P10	Application of UV Curable Siloxane Materials Bearing Covalently Bonded Luminophores as Color Converting Layers for Blue Diodes
Gaikova Elizaveta	P11	Novel Triazine-Benzothiadiazole Luminophores: Design, Synthesis and Optical Characterization
Gulenkov Danila	P12	Charge Carrier Mobility in Organic Materials with Correlated Disorder A Comparative Analysis of Microscopic Models and Effective Temperature Concept
Kevreva Maria	P13	Conjugated Polymer Composites as Promising Hole-Transport Materials for Stable and Efficient Perovskite Solar Cells
Kiy Nikita	P14	Study of the Influence of Deposition Parameters on the Semiconductor Properties of [1]Benzothieno[3,2-b][1]Benzothiophene Derivatives
Stakanova Daria	P15	Ortho-Substituent Effects in 2,1,3-benzothiadiazole-phenylene Systems

Poster session 2

Tuesday, September 15, 16:15

Fedorenko Roman	P16	Fabrication and Characterization of Blue OLEDs Based on Novel Multiple Resonance Diindolophenazine Derivatives
Kobeleva Elena	P17	Volatile Additive for Morphology Modification of Acceptors in the Active Layer of Organic Solar Cells
Kuleshov Bogdan	P18	EGOFET Multi-Sensor Device Design for Metal Detection in Aqueous Solutions
Kuzmin Yury	P19	MR-TADF Emitters Based On Quinolino[3,2,1-de]Acridine-5,9-Dione (QAO)
Lavrinenko Igor	P20	Cationic Iridium Complexes with Carboranyl-Derived Ligands for OLED Applications
Li Xiaodong	P21	Superior Impact Resistance in Bionic Nanocellulose Composite Supramolecular Elastomers via Multiple Hydrogen Bonding Interactions
Mikhailov Maxim	P22	Synthesis of Diindolophenazine Derivatives, Expansion of the Range of Fluorophores for the Creation of Blue OSDs
Molchanov Ivan	P23	Carbon-Based Additives for Modifying the Active Layer and Electrode Interfaces in Organic Solar Cells
Moseev Timofey	P24	Synthesis of Bipyridine Ligand Systems Containing Thiocarborane Species
Polyakov Roman	P25	Copolymer Structure Determination of Carbazole- and Triazinecontaining Styrene Monomers Through Copolymerization Kinetic Study Analysis
Semyonov Svyatoslav	P26	Synthesis and Characterization of a Series of Alkynylphosphine Sulfide Ligands
Sorokina Ekaterina	P27	Controlled Architecture of BTBT-Grafted Copolymers via Wittig, Hydrosilylation, and Click Chemistry: Towards Functional Receptor Layers
Steparuk Alexander	P28	Organic Photosensitizers Based on Indolo[3,2-b]carbazole with an A- π -D- π -A structure for Dye-Sensitized Solar Cells
Titova Yaroslava	P29	Semiconductor Properties of Novel Highly Soluble 2,7-diphenyl-[1]benzothieno[3,2-b][1]benzothiophene Derivative in Organic Field Effect Transistors
Zolotov Mikhail	P30	Donor–Acceptor Conjugated Polymers Absorbing in the Second Near-Infrared Transparency Window for Biomedical Applications

Tutorial lectures

Mechanisms of Catalytic Reactions in Organic Synthesis: How to Discover or Improve the Catalyst?

V.P. Ananikov*

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Mechanistic analysis is frequently treated as a *post hoc* explanation of a successful catalytic reaction. A more productive strategy is to use mechanism prospectively: to identify the catalytically competent states, determine how they interconvert under reaction conditions, and then redesign the system around the rate- and selectivity-determining events. This approach is especially important because the “catalyst” introduced into a flask is often only a precursor to a dynamic ensemble of molecular complexes, clusters, nanoparticles, ligand-free species and off-cycle reservoirs.

Recent studies illustrate three complementary consequences of this view. First, Au(I) and Cu(I) systems bearing phosphine or N-heterocyclic carbene ligands undergo rapid metal–ligand bond cleavage and generate reaction-dependent “cocktails” of species¹. The ligand may promote, inhibit or effectively disappear from the operative pathway; therefore, ligand optimization without identifying the dominant catalytic state can be misleading. Second, adaptive dynamic homogeneous Ni catalysis uses controlled self-adjustment rather than suppression of catalyst evolution. Under visible-light-driven redox conditions, the catalytic system responds to the nucleophile and enables multiple C(sp²)–heteroatom and C–C bond-forming reactions under predictable conditions². Third, mechanistic reasoning can reveal that catalyst modification is not always the correct solution. High-temperature solution chemistry can provide direct access to transformations with activation barriers of 50–70 kcal mol^{−1}, as demonstrated by kinetic measurements and DFT analysis of pyrazole isomerization³. Changing the accessible energy regime may thus open reaction space that conventional catalyst screening cannot reach.

Together, these examples suggest a practical workflow for catalyst discovery and improvement: establish catalyst speciation and its time evolution; identify whether activity is molecular, nanoscale or distributed across several channels; connect each state with kinetic and selectivity data; and only then decide whether to stabilize one species, accelerate productive interconversion, suppress deactivation, or redesign the activation mode. Operando spectroscopy and mass spectrometry, microscopy, poisoning and additive experiments, kinetic analysis, and computation should be used as mutually constraining tools rather than as isolated proofs. The central conclusion is that an improved catalyst is not necessarily the most stable or structurally elegant complex. It is the catalytic system whose dynamic response is matched to the mechanism and to the chemical task.

¹ Grudova M.V., Galushko A.S., Skuratovich V.A., Nakhatova A.O., Ilyushenkova V.V., Chernyshev V.M., Ananikov V.P. *Inorg. Chem. Front.* 2026, **13**, 4162–4174. DOI: 10.1039/D5QI02569A

² Ghosh I., Shlapakov N., Karl T.A., Düker J., Nikitin M., Burykina J.V., Ananikov V.P., König B. *Nature* 2023, **619**, 87–93. DOI: 10.1038/s41586-023-06087-4

³ Shaydullin R.R., Galushko A.S., Ilyushenkova V.V., Vlasova Y.S., Ananikov V.P. *Chem. Sci.* 2025, **16**, 5289–5298. DOI: 10.1039/D4SC08243E

**Luminescent Materials Based on Lanthanide Coordination Compounds - Synthesis,
Energy Transfer and Prospects for Practical Applications**

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Luminescent compounds of trivalent lanthanides are among the most extensively studied classes of coordination compounds used as luminescent materials. The luminescence of lanthanide ions covers the spectral range from the visible to the near-infrared. Narrow emission lines are observed, which accounts for the unique properties of these phosphors. This presentation will review the history of the use of lanthanide derivatives as emission layers in organic light-emitting devices. The specific features of the luminescence mechanisms of such compounds will be discussed in detail, as well as the experimental methods used to investigate these properties.

This work was supported by RSF (project № 25-13-00399).

Organic Semiconductors for Space Applications: Modelling Intrinsic Photostability and Radiation Resilience Based on Structure Descriptors

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In this report, we will discuss the results of our systematic study of a broad panel (>250 structures) of conjugated polymersⁱ and small molecules, including fullerene derivativesⁱⁱ [2] and non-fullerene acceptors (NFAs), in the context of their stability with respect to light and gamma rays. Important correlations between the materials' stability, their chemical compositions and molecular structures will be presented. The first prognostic model enabling an accurate prediction of photostability of arbitrary chosen conjugated polymer structures will be introduced, and the guidelines for rational design of new absorber materials for stable and efficient organic photovoltaics will be outlined.

This work was supported by Russian Science Foundation (project 25-13-00235).

ⁱ P. M. Kuznetsov, E. A. Komissarova, S. A. Kuklin, T. N. Khokhlova, P. G. Novkina, R. M. Khisamov, I. S. Zhidkov, O. A. Kraevaya, A. F. Shestakov, P. A. Troshin. *Adv. Energy Mater.*, 2025, e01179. DOI: 10.1002/aenm.202501179

ⁱⁱ I. V. Martynov, A. V. Mumyatov, L. G. Gutsev, L. N. Inasaridze, A. V. Kulikov, P. A. Troshin. *Adv. Funct. Mater.*, 2023, **33**, 2301637. DOI: 10.1002/adfm.202301637

Vertical Organic Field-Effect Transistors: Fundamentals and Current Trends

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Vertical Organic Field-Effect Transistors (VOFETs) have emerged as a compelling alternative to conventional planar organic transistors, addressing fundamental limitations in channel length scaling, current density, and operating voltage. This tutorial lecture provides a comprehensive overview of the operating principles, device architectures, and recent advances in VOFET technology.

Unlike planar OFETs, where the channel length is defined lithographically (typically in the micron range), VOFETs exploit the organic semiconductor film thickness (tens to hundreds of nanometers) as the vertical channel, enabling ultrashort channels and current densities exceeding 0.5 A/cm^2 at ultra-low voltages. Two complementary mechanisms govern vertical charge modulation: virtual contact formation (gate-tunable Schottky barrier at the source interface) and bulk conductivity modulation. The transparency of the source electrode to the electric field constitutes the central engineering challenge.

The lecture traces the evolution of transparent and nanostructured source electrodes — from block-copolymer self-assembled patterns and metallic nanowire networks to rolled-up nanomembrane architectures, which provide strain-engineered 3D electrodes with edge-dominated injection. Key results from our group anchor the discussion: the rolled-up nanomembrane VOFET platform demonstrating multi-sensing capability (temperature, magnetic field, and illumination) in a single device¹; the integration of VOFETs with optoelectronic functions showing on/off ratios up to 10^5 ²; the critical comparison of planar versus vertical technologies for flexible electronics³; and the recent electrolyte-gated vertical transistor enabling photo-switching⁴. A comprehensive review of vertical electrolyte-gated transistors, covering structures, materials, integration, and applications, has also recently been published⁵.

The lecture concludes with an outlook on the challenges — contact engineering, long-term operational stability, and circuit-level integration — that define the frontier of vertical organic electronics.

The author gratefully acknowledges the financial support from FAPESP (2025/25075-0; 2023/09820-2)

¹ Nawaz, A.; Mercés, L.; de Andrade, D.M.; Camargo, D.H.S.; Bufon, C.C.B. *Nature Communications*, **2020**, 11, 841.

² de Oliveira, R.F.; Mercés, L.; Vello, T.P.; Bufon, C.C.B. *Organic Electronics*, **2016**, 31, 217.

³ Nawaz, A.; Mercés, L.; Ferro, L.M.M.; Sonar, P.; Bufon, C.C.B. *Advanced Materials*, **2023**, 35(11), 2204804.

⁴ Vieira, D.H.; Nogueira, G.L.; Mercés, L.; Bufon, C.C.B.; Alves, N. *Advanced Electronic Materials*, **2024**, 6, 2300562.

⁵ Bufon, C.C.B. et al. *Advanced Electronic Materials*, **2025**, 11(11), 2400955.

How does OLED work?

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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. Nowadays, OLEDs is a mature technology, gradually replacing traditional LCD technology. Despite of great progress in the OLEDs, a number of challenges should be addressed to fully realize the potential of organic light-emitting devices, specifically, the energy efficiency, color purity and lifetime. On the other hand, the OLED structure should as simple as possible to provide low production cost.

This tutorial is focused on the basics of OLEDs and addresses the latest achievements and unsolved problems in the field. We start with the simplest a few layer OLED structure and analyze the reasons for its poor efficiency. The OLED generations are briefly reviewed: 1st-gen or fluorescent OLEDs with limited to 25% internal quantum efficiency (IQE) because of singlet-only utilization; 2nd-gen or phosphorescent OLEDs, achieving 100% IQE via heavy metals, though unstable for the blue range; 3rd-gen or TADF OLEDs, which harvest 100% of excitons without heavy metals by thermally converting triplets into singlets; and finally 4th-gen OLEDs based on novel concepts, specifically inverse TADF, hyperfluorescence and radical emitters.

The OLED efficiency metrics (IQE, EQE, energy efficiency, etc.) and key electrophysical processes in OLED are reviewed, including charge injection and transport, charge trapping and recombination, exciton generation and harvesting, spin statistics.

We review the two OLED technologies based on vacuum thermal evaporation of small molecules (industrial), which maximizes stability and efficiency through precise thickness control and high purity, and solution processing (not yet industrial), which can drastically lower costs and scales easily for large-area displays despite potential trade-offs in film purity. The pro and contra of these technologies are discussed.

The most promising concepts and materials for 4th-gen OLEDs are presented, specifically multiresonance emitters combining high efficiency and extremely narrowband emission.

The work was supported by Russian Science Foundation (project #24-49-02038).

Advances in Metal-Containing Luminophores: Thermally Activated Delayed Fluorescence (TADF)

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Metal TADF (thermally activated delayed fluorescence) emitters, which are broadly defined as luminophores incorporating a d-block metal, have emerged as an increasingly important class of emissive materials for application in organic light-emitting diode technology.¹ These molecular systems offer a distinctive photophysical properties, for instance, metal TADF complexes can exhibit exceptionally short delayed-fluorescence lifetimes, typically on the order of 0.1–10 μ s, together with efficient intersystem crossing (ISC) and reverse intersystem crossing (rISC) several orders faster compared to organic TADF emitters. Other commonly reported characteristics include exceptionally fast prompt fluorescence on a picosecond time-scale, albeit very weak, and pronounced temperature-dependent emission behaviour for the dominant delayed emission. Such a temperature dependent behaviour results in the fine balance/coexistence of TADF and phosphorescence in metal complexes. Although such dual and tri-luminescence are not universally observed across all metal-containing TADF systems, those becoming of particular interest for bioimaging and temperature/pressure-sensitive paints development for aerospace industry.

We will discuss photophysical mechanisms responsible for TADF in organometallic complexes, with both experimental and computational approaches being employed to investigate the excited-state dynamics and thermal up-conversion processes across 3d-metal block and followed by a range of heavier metal centres including Pd(II), Pt(II), Au(I)/Au(III), and Zr(IV) compounds. Also, a particular attention will be focussed on emerging two-coordinate coinage metal complexes with linear geometry L–M–X (L = carbene and X = anionic ligand, M = copper, silver or gold) that have recently emerged as a new class of strongly photoemissive TADF materials – Carbene Metal Amides (CMA).² We will discuss the advances in CMA molecular design to cover the full visible spectrum and near-IR region (up to 850 nm). A comprehensive comparison across various classes of emitters will be based on the bond dissociation energies of the metal–ligand bond and on intra- and intermolecular contacts in the CMA emitter, to demonstrate molecular designs that lead to the best photophysical and OLED performance and suitable candidates for application in nonlinear photonics.

This work was supported by the Royal Society (grant nos. URF R1 180288, RGF EA 181008, URF R231014), EPSRC (grant codes EP/K039547/1 and APP46952).

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Charge Transport Collapse in Organic Semiconductors: Competing Views and Frameworks

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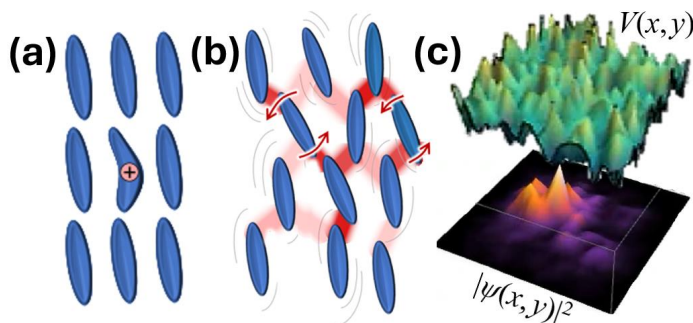


Fig. 1. Schematic representation of a small polaron (a) and a molecular crystal with dynamic disorder (b); Anderson localization of charge-carrier wavefunction ψ in a 2D crystal with a random potential V (c).

Crystalline organic semiconductors (OSCs) are a zoo of various physical phenomena, from polymorphism to the (hypothesized as possible) room-temperature superconductivity. This, on one hand, makes them extremely flexible and favorable for molecular design, while on the other hand, obscures successful routes to attaining a number of practically important characteristics in them, including charge-carrier mobility, μ . In fact, there is no ultimate consensus on what actually limits μ in the most appealing OSCs with the so-called band-like mobilities above $\sim 1 \text{ cm}^2/\text{Vs}$, making engineering of even higher- μ OSCs a challenging task. That said, the success of molecular design or screening of high- μ OSCs depends on the correct understanding of charge transport physics therein. In this tutorial, I will elucidate different suspected “killers” of efficient transport, mainly focusing on polaronic effects¹ (Fig. 1a) and the dynamic disorder² (Fig. 1b). Both effects stem from the “softness” of molecular crystals formed by weakly-bound molecules, with their deformations or thermal relative motions resulting in a strong electron-phonon interaction³. I will portray the corresponding competing theories^{i,ii}, both of which predict a band-like mobility, however, from completely different physics. Along the way, I will review the fundamentals of such exciting phenomena as Anderson localization (Fig. 1c) and ballistic quantum transport. Finally, I will give several examples of how one should and how one should not calculate the mobility in OSCs.

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

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SIMS Analysis of Multilayer Organic/Inorganic Structures

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Secondary ion mass spectrometry (SIMS) is the destructive technique for studying the elemental and molecular composition of multilayer optoelectronic devices in the bulk, down to the substrate. It is well known that all commercially relevant ‘organic electronic’ devices are in fact hybrid organic-inorganic (hetero-)structures comprising active layers of small molecules (or polymers) and various functional inorganic components, such as electrode metals, transporting or blocking layers, optical spacers, etc.

The depth profiling of such structures requires a combination of two (previously separated) SIMS modes: static analysis of the surface molecular composition and dynamic layer-by-layer elemental analysis. To achieve this, modern setups utilize two ion guns, each performing distinct functions: a probing beam and a sputtering beam. The parameters of each of them should independently be optimized to get both the detectable secondary ion yield over a wide range of atomic masses with minimal fragmentation of molecules, and the sputtering process with a minimal damaged layer. The latter process requires a significantly higher amplitude and current density than the probing beams, and hence the formation of a damaged layer, where the complete destruction of the analyzed molecules into fragments and atoms occurs, becomes nearly inevitable.

In this talk, the advantages and disadvantages of ToF-SIMS profiling for analysis of physicochemical processes running inside multilayer organic/inorganic structures of interest for application in organic electronics are described. An overview of some of our results obtained on typical functional materials such as phthalocyanines, fullerenes, LiF and MoO₃ is presented¹.

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Standards and Guidelines for Good Practice in Organic Electronics: Where Do They Come from and Why Do We Need Them?

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Organic electronics develops very fast due to elaboration of novel functional materials, improving their processing techniques and appearance of new device architectures. Such development requires that many researchers of this multidisciplinary field working in different countries in the world should understand each other in terms of nomenclature of the materials, terminology of the phenomena investigated and as well as comparability of the results obtained. This tutorial lecture aims to cover some main standards and guidelines for good practice in organic electronics and highlight the sources where they can be found.

Terminology and nomenclature for different materials is elaborated for many years by the corresponding experts in the International Union for Pure and Applied Chemistry (IUPAC). Nowadays it has a collection of Color Books, which cover different aspects of chemistry and related phenomenon.¹ Since organic electronic materials includes organic molecules and polymers, the most important are **Blue book** and **Purple Book** named as “Nomenclature of Organic Chemistry” and “Compendium of Polymer Terminology and Nomenclature”, respectively. General “Compendium of Chemical Terminology” is covered by **Gold Book**, which is available online as a free interactive version.² For those who are new in the field, several **Brief Guides** for Organic, Inorganic and Polymer Nomenclature are available and the new version are elaborated.³

The IUPAC publish Technical Reports and Recommendations in the journal “Pure and Applied Chemistry”. One of the recent publications important for organic electronics is “*Glossary of terms relating to electronic, photonic and magnetic properties of polymers (IUPAC Recommendations 2021)*”.⁴ The experts continue to work on various aspects of terminology and nomenclature relevant to organic electronics and the new recommendations are to be published soon.

One of the most important standards for organic light emitting devices is CIE 1931 color space. It was developed by the International Commission on Illumination (CIE) in 1931 and widely used for the estimation of the color purity, which define the relationship between the visible spectrum and human color vision. Since that time some other corrections have been elaborated, but still CIE 1931 color space is the most widely used.

For estimation of the device efficiency in organic photovoltaics the most important is the standard 1.5G, implying the power of 100 mW/cm² under the solar light spectrum appeared to the earth surface passed through 1.5 air mass atmosphere. Last but not less is testing of the device efficiency in the certified laboratories under the standard conditions. These and other examples of the standardization will be considered.

This work was supported by Ministry of Science and Higher Education of the Russian Federation (State task FFMSM-2024-0003).

¹ <https://iupac.org/what-we-do/books/>

² <https://goldbook.iupac.org/>

³ <https://iupac.org/what-we-do/nomenclature/brief-guides/>

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Invited lectures

1,4-Diazatriphenylene and Its Hetero-Fused Analogues: Synthesis and Applications

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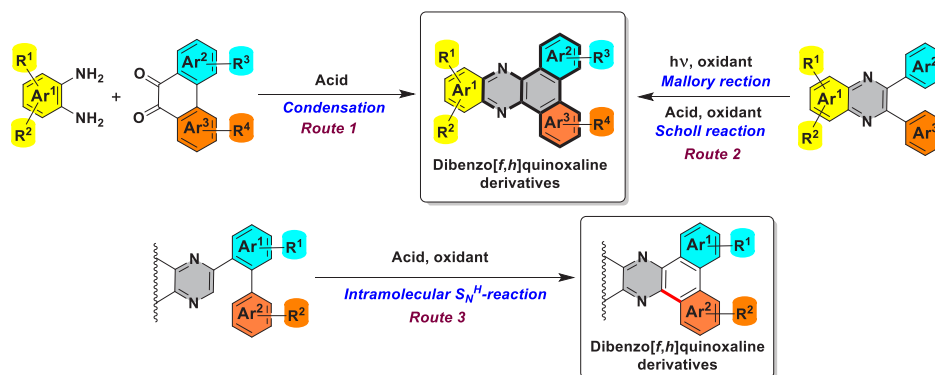
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Over the past three decades, polycyclic aromatic hydrocarbons have gained widespread use in materials chemistry, organic electronics, and the design of chemosensors and molecular probes for biomedical applications.^{i,ii} In particular, 1,4-diazatriphenylene, also known as dibenzo[*f,h*]quinoxaline, along with its heteroannelated analogs, is regarded as a promising scaffold for developing functional charge-transport and light-emitting materials.

The most common method for constructing the 1,4-diazatriphenylene skeleton is through condensation reactions (Route 1). Another less common synthetic approach involves intramolecular cyclizations of 2,3-di(het)aryl-substituted pyrazine derivatives using oxidative photocyclization (*Mallory reaction*) or intramolecular cyclodehydrogenation with chemical oxidants under acidic conditions (*Scholl reaction*) (Route 2). This report will particularly focus on the use of the intramolecular nucleophilic aromatic hydrogen substitution reaction (S_N^H -reaction) involving 2-bis(het)aryl-substituted 1,4-diazine derivatives (Route 3).

In addition, data on the photophysical and electrochemical properties of the resulting products, as well as their potential applications as organic semiconductor materials, will be discussed.



This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project No. 124020500039-0).

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Functionalized Polyfluorenes for Optoelectronics and Medicine

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Due to their luminescent and charge-transport properties, polyfluorenes and their copolymers find wide application in optoelectronics as light-emitting and photoactive materials. For use in optoelectronic devices, particularly organic light-emitting diodes (OLEDs), it is necessary to ensure a sufficiently high and balanced mobility of electrons and holes injected into the light-emitting polymer layer. To achieve this, electron-acceptor units must be introduced into the polyfluorene structure to facilitate electron transport between molecules, as the electron conductivity of polyfluorenes is significantly lower than their hole conductivity. In this study, a series of copolyfluorenes with dicyanostilbene and phenanthrene-9,10-dicarbonitrile moieties were prepared via polycondensation via the Suzuki reaction mechanism. For OLEDs with these copolyfluorenes as light-emitting material, the highest electroluminescence brightness (11000 cd/m²) and the lowest turn-on voltage (3.1 V) were achieved.

To create a chemosensor for β -lactamase secreted by tuberculosis patients, a cephalosporin moiety was introduced into the end group of copolyfluorene containing 2.5 mol% dicyanostilbene. It has been shown that cleavage of the cephalosporin fragment by β -lactamase leads to a change in the photoluminescence spectrum with a shift to the yellow region (Fig. 1).

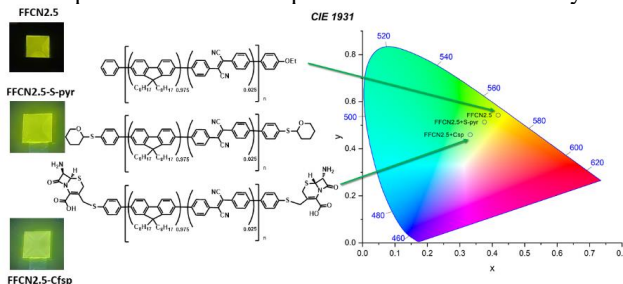


Fig. 1. Change in photoluminescence color upon cleavage of the terminal cephalosporin fragment.

A simplified in situ method for producing TADF polymers has been developed, in which TADF-active tricarbazole-triazine fragments are formed directly during polymer chain growth. The method is based on Suzuki polycondensation using readily available monomers that do not exhibit TADF properties individually. The use of the stable PEPPSI-IPr catalyst allowed for open-air synthesis, eliminating the need for an inert atmosphere.

The inclusion of bis(4-bromobenzyl)dimethylsilane in the polymer ensured high solubility in toluene and chlorobenzene and significantly increased the material's resistance to concentration quenching—luminescence remains stable up to 50 wt% doping (unlike its silicon-free counterpart, where quenching begins at 10 wt%). The resulting polymer is characterized by a small singlet-triplet splitting of $\Delta E_{ST} = 0.045$ eV, a photoluminescence quantum yield of 30%, and a delayed component lifetime of 2.3 μ s. OLED devices created on the basis of this polymer demonstrate a maximum brightness of 4000 cd/m², an external quantum yield of 13%, and an electroluminescence peak at 500 nm.

Diazafluorenes for Organic Optoelectronics and Sensorics

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Linear conjugated small molecules and polymers are widely used in organic optoelectronics as hole semiconductors and luminophores. Among them, fluorene-containing materials were previously extensively used in organic light-emitting diodes, transistors and solar cells.¹ However, their functionalized counterparts - diazafluorenes have been poorly explored though their nitrogen atoms enhance electron affinity and may improve electron transport.^{2,3,4} Moreover, 4,5-diazafluorene-containing materials are promising for sensorics because of the N-coordination and protonation opportunities.⁵

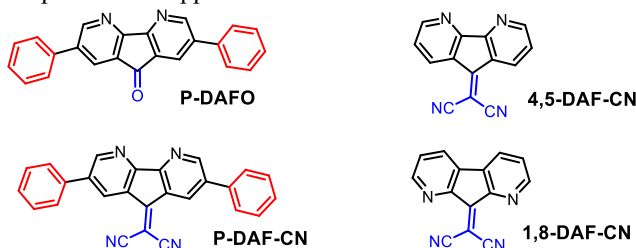


Fig. 1. Chemical structures of a representative series of diazafluorene(on)e-based semiconductors.

Here, we discuss design, synthesis and functional properties of a series of both 4,5- and 1,8-diazafluorene-derivatives containing different donor/acceptor groups. We have optimized the synthesis of diazafluorenylidene via Knoevenagel condensation reactions.⁶ Crystal structures of all the materials were solved by X-ray diffraction revealing extensive π -stacking interactions leading to anisotropic charge transfer pathways.² 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. The key molecular design ideas for good electron transport in these systems are the tuning of molecular dipole moments and crystal packing. The practical potential of fabricated devices was demonstrated by their sensor response toward sub-ppm concentrations of hydrogen sulfide. Therefore, both 4,5- and 1,8-diazafluorene-based materials are promising electron semiconductors for organic optoelectronics and sensorics.

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

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Towards Elastic Electronics: Light-Driven Fabrication of Stretchable Nanocomposites

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Stretchable electronics, as a key enabler for next-generation wearables, require conductors that remain functional under mechanical strain. Percolating silver nanowire (AgNW) networks are a promising strategy to achieve this because they combine metallic conductivity with mechanical compliance. However, when deposited on elastic substrates, these networks often fail due to delamination and cracking. Embedding AgNWs beneath the surface offers an effective solution, particularly with light-based processing as an elegant and controllable means to achieve this. Our laser-integration approach exploits the melt pool and Marangoni convection to draw nanomaterials into a polymer surface¹ and is broadly applicable provided the polymer substrate is a thermoplastic². Recently, this approach was extended to AgNW networks³. However, this mechanism (laser embedding via percolation interlocking) was not applicable beyond thermoplastics: cross-linked elastomers do not melt, precluding melt pool formation⁴. In this lecture, we will discuss how this limitation can be overcome. In a side-chain-crystalline cross-linked network (bistable adhesive polymer, BAP⁵), a reversible ~ 30 °C semicrystalline-to-amorphous transition provides a laser-addressable softening channel while the permanent network stays intact. Upon laser irradiation, individual AgNWs induce localized softening, evidenced by an optical halo corresponding to the transition isotherm, and are driven beneath the surface, as confirmed by atomic force microscopy (Fig. 1). Control experiments on bare BAP confirm a nanowire-mediated photothermal mechanism. This work establishes a foundation for full-network integration with simultaneous junction welding, ultimately advancing toward autonomous laser-based platforms for the manufacturing of elastic electronics.

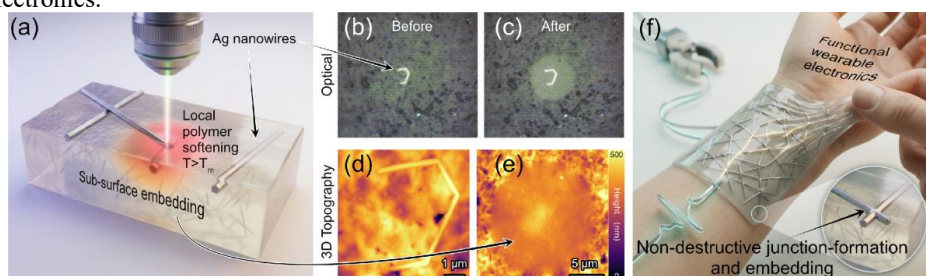


Fig. 1. Laser-driven sub-surface embedding of an AgNW into BAP: (a) mechanism; (b, c) optical images and (d, e) AFM images before/after irradiation showing the softening halo and the wire on the surface before and embedded after laser processing. (f) Our long-term aim is to bring robust, inexpensive, stretchable electronics within reach.

This work was supported by RSF (project № 26-13-00500).

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Interfacial Engineering of Perovskite Solar Cells

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Our systematic investigation of interfacial issues in perovskite solar cells covers film formation kinetics, carrier transport in 2D perovskites, and device stability. In-situ optical characterization during blade coating revealed that sulfonium cations promote intermediate conversion, solvent engineering reduces trap states, and spacer cation tuning releases residual strain, correlating crystallization rate with stress. For quasi-2D perovskites, slow post-annealing facilitates energy transfer and carrier transport, while designed slightly-displaced Dion–Jacobson materials achieve over 6000 h operational stability. To synergize stability and efficiency, we constructed 2D/3D heterostructures via preformed 2D intermediates, yielding vertically aligned α -FAPbI₃ with improved orientation and passivation. This delivered 27.4% device efficiency and 23.58% module efficiency (13.01 cm²), with >95% retention after 1100 h MPP tracking and 1700 h damp-heat testing (85% RH, 85 °C).

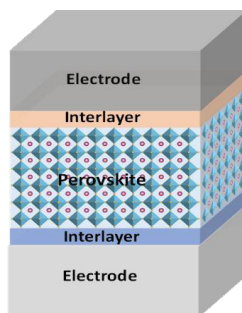


Fig. 1. Scheme of device structure of perovskite solar cells.

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Recent Achievements in The Development and Scaling of Perovskite Modules

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Perovskite photovoltaics (PV) represent a transformative thin-film technology, yet bridging the gap between small-scale lab devices and commercially viable, large-area modules requires overcoming critical bottlenecks in operational stability and reproducible ambient-air scalable processing.

At IRITALY Trading Company S.r.l. (ITC), recent achievements focus on advancing ultra-stable, low-CAPEX/OPEX perovskite PV solutions manufactured via ambient-air solution processing. Central to our technological progress is a novel 3D/2D co-crystal engineering strategy recently published in *Nature Energy*ⁱ. By engineering a tailored two-dimensional perovskite interlayer, we effectively suppress interfacial recombination and structural degradation, overcoming the historic "instability bottleneck" of perovskites. Large-area solar modules fabricated via this method demonstrate exceptional, certified durability across rigorous terrestrial and space-simulated stress tests: retaining >95% initial efficiency after >5,000 h of continuous 1-sun light soaking, >98% after >1,000 h of intense UV exposure at maximum power point, and >91% after >5,000 h of damp-heat stress at 85 °C and 65% relative humidity. Building upon these large-area, ultra-stable PV modules, ITC is expanding technology applications within the EIC Pathfinder SUNPEROM project. SUNPEROM aims to revolutionize decentralized clean energy by coupling high-voltage perovskite module architectures directly with electrochemical conversion platforms for standalone Solar-to-X applications—specifically converting abundant atmospheric CO₂ into green methanol and value-added chemicals without relying on traditional electricity grids. This presentation details our advances in module scaling, co-crystal passivation, ambient processing, and the role of resilient perovskites in driving next-generation solar-driven electrochemical platforms.

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Biosensors Based on Electrolyte-Gated Organic Field-Effect Transistors for the Specific Antibody Detection

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Invasive pulmonary aspergillosis (IPA) is a dangerous fungal infection. At the initial stages, IPA has no characteristic clinical manifestations, therefore its early diagnosis is an essential problem. The important markers that allow fungal infection diagnostics are galactomannan (GM) and β -D-glucans (BDG), polysaccharide antigens that exists mainly in the cell wall of *Aspergillus* fungi. Currently, the main method for GM and BDG determination in biological fluids is enzyme-linked immunosorbent assay (ELISA)ⁱ. The analysis can be carried out only under laboratory conditions since it requires the use of washers and large fluid flow. The development of biosensors opens new horizons in biomarker detection. Electrolyte-gated organic field-effect transistors (EGOFET) are a promising platform for ultrasensitive, fast and reliable detection of biological molecules by low cost, point-of-care electronic sensorsⁱⁱ.

We used previously developed method of functionalization of the C8-BTBT/PS EGOFET surface with biotin receptorsⁱⁱⁱ. The biosensor principle is based on biotin-streptavidin interaction on the EGOFET platform and it is well-proven for different analytes^{iv}. The recognition elements in the sensor architecture are biotinylated oligosaccharides (GM and BDG), that form the biotin-streptavidin based sandwich on EGOFET surface, and specifically bind the monoclonal antibodies (7B8, 5H5 and 1D2). However, the EGOFET recognition layer composition was earlier optimized for influenza A virus detection, here the biorecognition surface was adapted. The 20% BTBT-biotin containing recognition layer provides the better accuracy of antibody detection. In order to improve the formation of recognition layer new BTBT-biotin compound designed and synthesized, containing ethoxy-groups in large spacer towards biotin fragment. Such chemical composition of functional compound provides better organization of the thin monolayer film of BTBT-dimer and BTBT-biotin (recognition layer similar to described in [3]) due to more hydrophilic fragment, connected to biotin in BTBT-biotin. The most relevant region of antibody concentration determination is below 50 ng/mL – in order to detect the disease IPA at the earliest stages. Here the region 1.69-50 ng/mL was investigated. The detection limits of 7B8, 5H5 and 1D2 by the corresponding oligosaccharides are equal 4 ng/mL.

This work was supported by Ministry of Science and Higher Education of the Russian Federation (Contract FFSM- 2025-0001).

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ⁱⁱ E. Macchia and L. Torsi, "Biochemical Sensing" (Melville, New York, 2022), Chap. 5.

ⁱⁱⁱ E.Y. Poimanova et al. ACS Appl. Mater. Interfaces, 2022, **14**, 16462.

^{iv} E.Y. Poimanova et al. J. Mater. Chem. B, 2026, **14**, 2543

Photosensitive Organic-Inorganic Hybrid Materials for Gas Sensor Applications

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In this work, the optical characteristics and conductivity under photoactivation with visible light of hybrids based on nanocrystalline SnO₂ or In₂O₃ semiconductor matrixes and heteroleptic Ru(II) complex were studied. The heteroleptic Ru(II) complexes were prepared based on 1H-imidazo[4,5-f][1,10]phenanthroline and 2,2'-bipyridine ligands. Nanocrystalline semiconductor oxides were obtained by chemical precipitation with subsequent thermal annealing and characterized by XRD, SEM and single-point BET methods. The heteroleptic Ru(II) complexes as well as hybrid materials were characterized by time-resolved fluorescence and X-ray photoelectron spectroscopy. The results showed that the surface modification of SnO₂ nanoparticles with heteroleptic ruthenium complexes led to an increase in conductivity upon irradiation with light appropriate for absorption by organometallic complex. In the case of In₂O₃, the deposition of Ru (II) complexes resulted in a decrease in conductivity, apparently due to the special structure of the surface layer of the semiconductor. Synthesized organic–inorganic hybrid materials based on the nanocrystalline semiconductor oxide and Ru(II) heteroleptic complex demonstrated high sensitivity in gas detecting at room temperature under periodic illumination with blue light.

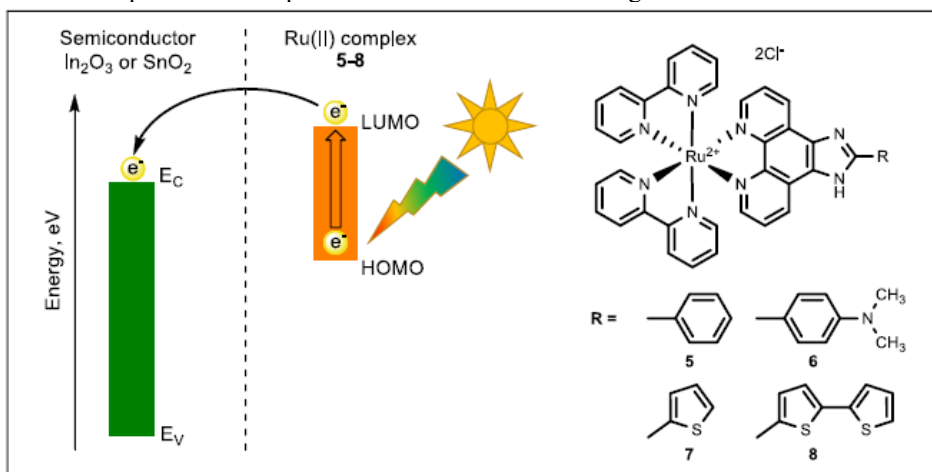


Fig. 1. Picture illustrating processes occurring after excitation of ruthenium (II) complexes **5-8** on the surface of SnO₂ or In₂O₃.

This work was supported by RSF (project № 25-73-20122).

Boron β -Diketonate–Arene Exciplexes: from Molecular Photophysics in Solution to Sensor Materials

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Bridging the gap between the photophysical properties of organic molecules in solution and their performance in bulk materials and devices remains a major challenge in many areas, including organic electronics. The pathway from fundamental studies of intermolecular interactions in the liquid phase to the development of solid-state sensor materials has been traced using boron difluoride β -diketonate^{i,ii} derivatives. The ability of boron difluoride β -diketonates to form exciplexes with arenes makes them promising molecular probes. The materials can be obtained, for example, by covalently attaching fluorophores to the surface of silica nanoparticles.

The primary focus in this study is placed on establishing the key mechanisms responsible for the non-radiative deactivation of excited states of the investigated class of molecules in solution. It was demonstrated that the dominant process involves changes in the molecular geometry upon excitation. This understanding allows for the design of non-fluorescent molecules where the non-radiative process dominates over the radiative oneⁱⁱⁱ.

The influence of electron-donating and electron-withdrawing substituents in a series of fluorophore derivatives on the efficiency of exciplex formation with arenes was investigated. Exciplex formation successfully competes with non-radiative deactivation. This provides a basis for the development of molecular probes that selectively activate ("turn on") luminescence upon interaction with aromatic compounds^{iv}. It is shown that the efficiency of such probe systems can be enhanced by transitioning to multichromophoric architectures. The transformation of the photophysical mechanisms identified in solution upon transfer to solid-state materials with covalently immobilized fluorophores was analysed. The obtained results reveal how molecular photophysical processes are modified upon immobilization on a solid-state surface and provide guidelines for the design of sensor materials with a controlled luminescence response.

This work was supported by Russian Science Foundation (grant no. 24-13-00443).

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Time-Resolved Spectroscopy for New Optoelectronic Materials Discovery

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On-demand selective photocontrol of electronic materials remains a holy grail of photochemistry. One approach to such control is through selective stimulation of materials' vibrational dynamics — vibrational control (VC). The phenomenon of electron-phonon interaction opens up an attractive practical applicability of VC: driving complex ultrafast chemical reactions with ultrafast pulses of infrared (IR) light and controlling excitations in photovoltaic materials. However, demonstrations of VC remains scarce in the literature and are only available for a limited range of solution-based model systems to study fundamental properties available via other spectroscopy techniques/modelling.ⁱ

In this work we developed a novel spectroscopy allowing VC in a broad range of optoelectronic materials including metal-halide perovskites (MHPs), photosensitive asymmetric nanogaps (PANs), organic single crystals, and organic photovoltaic blends. This spectroscopy is called photocurrent/photoluminescent vibrationally promoted electronic resonance spectroscopy (PC/PL VIPER, see Fig.1).ⁱⁱ

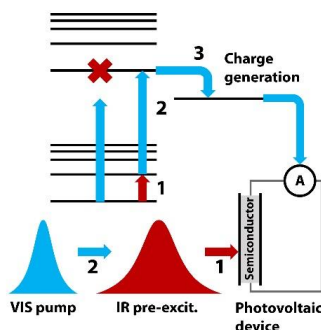


Fig. 1. PC-VIPER: (1) Vibrations of a semiconductors (SC) are pre-excited with an infrared (IR) pulse. (2) Electronic states are excited with a visible (VIS) pulse. (3) The electronic excitation is followed by charge generation and photocurrent detection within the device.

By applying PC/PL VIPER, we were able to untangle the complex dynamical picture of organic cation–inorganic framework coupling in MHPs, which appears to arise from stochastic sticking and unsticking of organic cations, mediated by cation–halide hydrogen bonding. We revealed symmetry breaking phenomena in organic rubrene single crystals. And finally, we achieved real VC control altering the photoexcitation path in a P3HT/O-IDFBR blend.

This work was supported by a grant for the support of research centers in the field of artificial intelligence, provided by the Ministry of Economic Development of the Russian Federation (subsidy agreement identifier No. 0000001313925P4E0002), and by an agreement with the National Research University Higher School of Economics dated June 23, 2025, No. 139-15-2025-009.

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Design and Multiscale Modelling of New Effective TADF-Luminophores

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Thermally activated delayed fluorescence (TADF) has emerged as a key mechanism for achieving nearly 100% internal quantum efficiency in organic light-emitting diodes (OLEDs). Conventional donor–acceptor (D–A) molecular architectures reduce the energy gap between the lowest excited singlet and triplet states, thereby promoting efficient reverse intersystem crossing and enhancing electroluminescence. However, these systems typically rely on relatively weak C–N donor–acceptor linkages, which may compromise their chemical and operational stability. In contrast, the multi-resonance TADF (MR-TADF) approach has proven highly effective in simultaneously achieving narrow emission spectra and high photoluminescence quantum yields. Nevertheless, most reported MR-TADF emitters incorporate boron atoms, whose high chemical reactivity presents challenges for material stability and practical device applications.

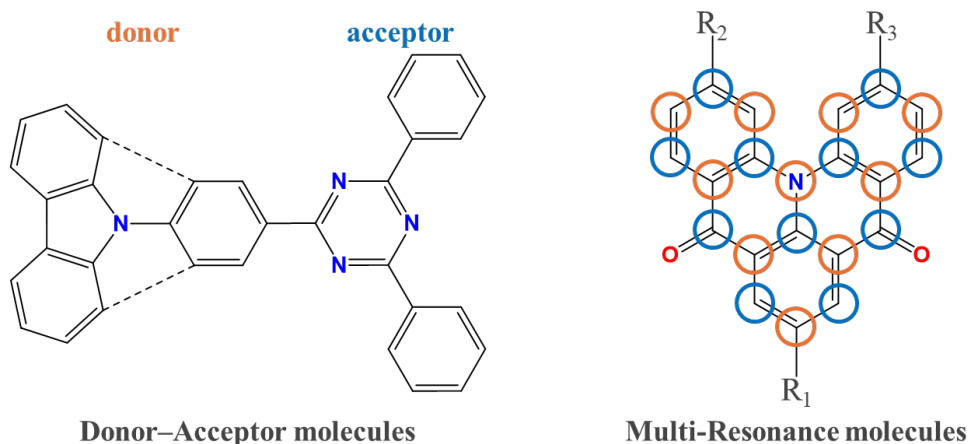


Fig. 1. Structures of studied TADF-luminophores and it's derivatives

Predictive theoretical modeling offers an efficient route for accelerating the discovery and rational design of high-performance OLED emitters. In this work, we present a multiscale computational framework for predicting the structural, energetic, and optical properties of both established and prospective TADF materials. The proposed methodology demonstrates high predictive accuracy and broad applicability to OLED material design. Furthermore, we introduce computational approaches for evaluating the chemical and structural stability of these compounds, providing additional guidance for the development of robust next-generation TADF emitters.

The work is supported by the Russian Science Foundation (project № 25-73-10304).

Modern In Situ Methods for Monitoring Supramolecular Structure Formation in Organic Semiconductors

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The performance of organic semiconductors is critically governed by the evolution of their supramolecular structure during film processing. Molecular packing, polymorphism, crystal orientation, and phase separation strongly influence charge transport, doping efficiency, and device performance. Consequently, understanding the kinetics of structure formation has become a key challenge in the rational design of organic electronic materials.

Recent advances in synchrotron radiation, high-brilliance X-ray sources, fast area detectors, and microfocused beams have enabled *operando* studies of structural evolution with unprecedented spatial and temporal resolution. Small- and wide-angle X-ray scattering (SAXS/WAXS), grazing-incidence WAXS (GIWAXS), and complementary methods now allow direct observation of nucleation, crystal growth, polymorphic transitions, molecular orientation, and hierarchical self-assembly during solution processing, solvent treatment, thermal annealing, and electrochemical doping. Examples will be presented demonstrating how in situ characterization reveals the mechanisms governing structure–property relationships in polymer semiconductors.

In particular, polymorphism in PBTTT with single-ether side chainsⁱ has been shown to produce two distinct supramolecular organizations—a liquid-crystalline phase with enhanced backbone planarization and π -stacking, and a crystalline phase exhibiting increased backbone torsion. These structural differences lead to markedly different doping efficiencies and charge transport, resulting in superior thermoelectric and electrochemical performance of the liquid-crystalline phase. Such studies highlight the importance of monitoring structural evolution in real time to understand how processing conditions determine the final electronic functionality.

The combination of time-resolved X-ray scattering with complementary techniques such as fast chip calorimetry provides a comprehensive multiscale picture of supramolecular structure formation. These methodologies offer powerful tools for optimizing processing protocols, controlling polymorphism and molecular ordering, and accelerating the development of high-performance organic semiconductors for flexible electronics.

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Oral talks

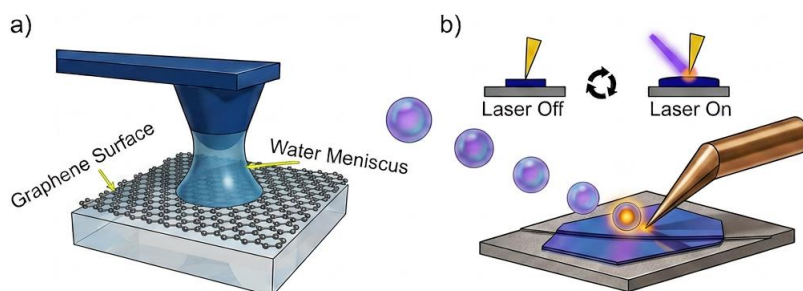
Advanced Nanoscale Surface Analysis of Materials for Flexible Electronics and Sensors

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Two-dimensional layered materials, and particularly graphene-based ones, are widely used in sensors and proof-of-concept flexible electronic devices due to their tunable electrical, mechanical, and chemical properties. Advancing these materials from laboratory demonstrations to real devices, as well as deepening their fundamental understanding, requires precise characterization of the surface state. Standard tools such as electron microscopy, photoelectron spectroscopy, and conventional atomic force microscopy (AFM) provide an essential baseline; however, they fall short for heterogeneous systems such as graphene oxide (GO) and reduced graphene oxide (rGO), where surface properties vary at the nanoscale. In this work, we present advanced AFM-based methods for mapping local chemistry and wettability with sub-micron resolution. AFM force spectroscopy is used to probe local variations in wettability, offering insights that conventional contact angle measurements lack the sensitivity to resolve nanoscale inhomogeneities (Fig. 1a). Complementary, Nano-Vis imaging visualizes optical absorption phenomena at the nanoscale, providing spatially resolved information on local chemical composition and bandgap across the surfaces (Fig. 1b).



Together with the micro- and nanoscale characterization methods already established within the research group, these updates form a comprehensive analytical toolkit that reveals structure–property relationships governing the performance of layered materials for optoelectronics.

This work was supported by RSF (project № 25-23-01236).

Pt(II) complexes with alkynylphosphine oxide ligands: variety of luminescent properties in polymeric films

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Pt(II) complexes are one of the most widely studied compounds worldwide due to their rich luminescent properties, including those arising from non-covalent interactions (Pt-Pt bonds). Besides obvious change of emission wavelength upon aggregation, these compounds can show AIE (aggregation-induced emission). This effect opposes widely known ACQ, aggregation-caused quenching, which is typical for the majority of luminophores, and thus can be interesting for OLED applications.¹

To achieve aggregation in Pt(II) complexes in non-solid environment, mixtures of “good-bad” solvents are used.² An alternative way is doping of polymeric films with target complex. In present work we study both approaches, using novel complexes **Pt0–Pt3** (Fig.1) as doping agents.

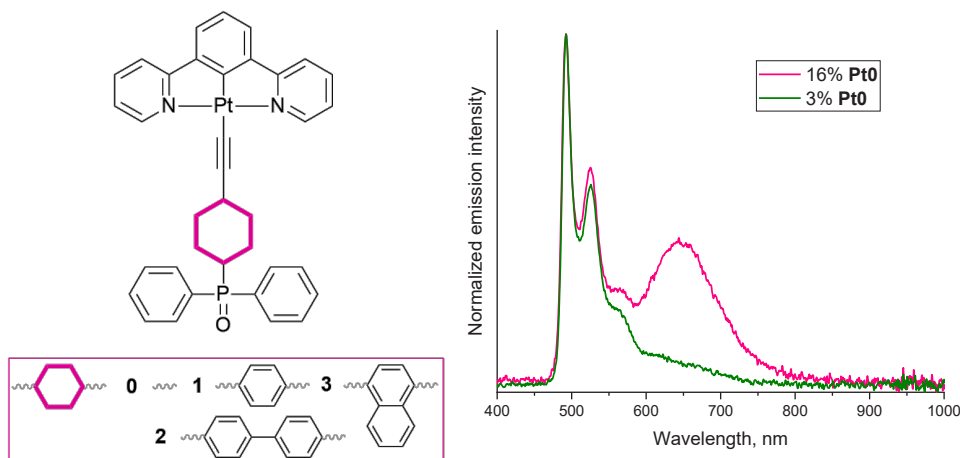


Fig. 1. (left) Complexes **Pt0–Pt3**, (right) emission spectra of PMMA films, doped with complex **Pt0** with different concentrations

The studied complexes' series were designed to combine two advantages: flat square-planar Pt(II) fragment, prone to aggregation, and phosphine oxide functional group, that can potentially improve electron-transport characteristics of emissive layer in OLED devices.³ Emission characteristics and their dependence on concentration of doping agents are discussed herein.

This work was supported by RSF (project № 24-13-00024). The authors thank Centres for Magnetic Resonance, for Optical and Laser Materials Research, for Chemical Analysis and Materials Research, and X-ray Diffraction Centres (Research Park of St Petersburg University) for providing the necessary equipment and analyses.

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D- π -A Structures Based on [1,2,4]triazolo[c]quinazolines: Multifunctional Fluorescent Molecules

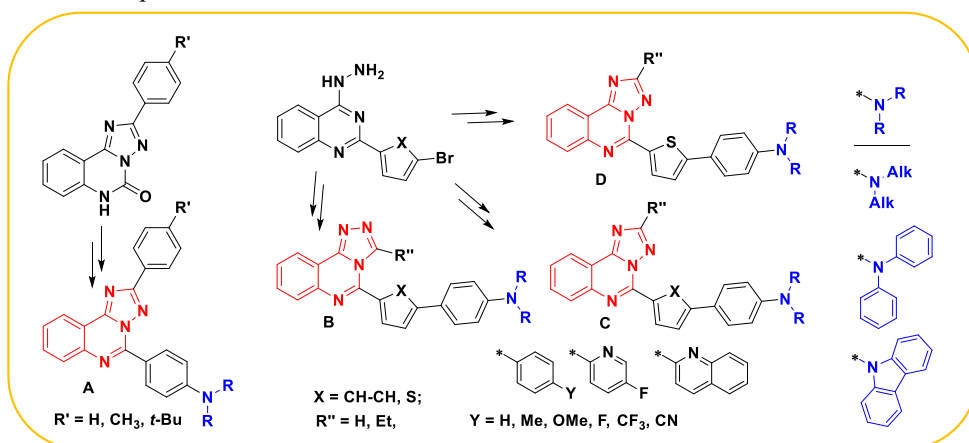
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Triazolo[c]quinazolines provide a promising molecular platform for various pharmaceutical applications and materials sciences¹.

Novel tricyclic fluorophores **A** were obtained from 2-aryl-[1,2,4]triazolo[1,5-*c*]quinazoline-5(6*H*)-ones through chlorodesoxygenation and subsequent Suzuki–Miyaura cross-coupling reactions². The synthetic approach to triazolo[c]quinazoline derivatives **B–D** is based on the condensation of 4-hydrazino-2-(5-bromothiophen-2-yl)quinazoline with various aryl(hetaryl) aldehydes, followed by oxidative cyclization with bromine at room temperature^{3,4} or condensation with orthoester and subsequent cross-coupling reactions with aminoarylboronic acids or their pinacol esters.



Some compounds exhibited pronounced fluorescence (over 95%) both in solution and the solid state. Moreover, they displayed solvatochromic properties and AIE activity.

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Synthesis of New Comb-Shaped Polymers Containing 2-undecyl-7-octyl-[1]benzothieno[3,2-b]benzothiophene Moieties

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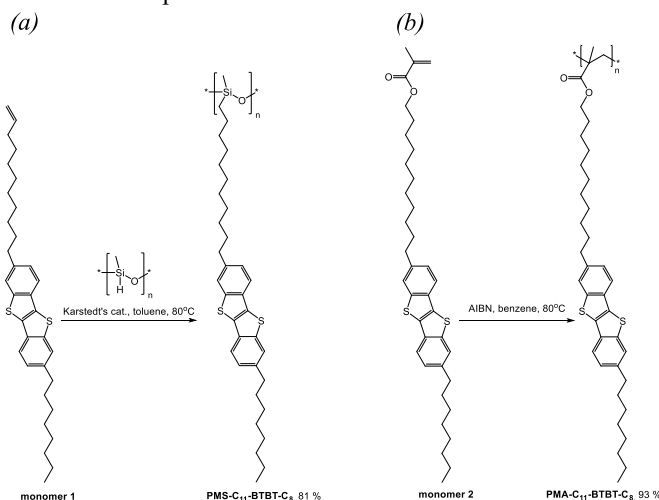
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The organic semiconductor materials can be used as active layers in different organic semiconducting devices¹. Currently, such materials can be used as ink in the microelectronic devices and forms active layer using modern printing methods².

In this work, two new comb-shaped polymers, **PMS-C₁₁-BTBT-C₈** and **PMA-C₁₁-BTBT-C₈**, containing 2-undecyl-7-octyl-[1]benzothieno[3,2-b]benzothiophene (Scheme 1) side groups attached to the polymethylsiloxane and polymethacrylate main chain, respectively, were synthesized for use as inks for printed microelectronics.



Scheme 1. Synthesis of target polymers: (a) – **PMS-C₁₁-BTBT-C₈**; (b) – **PMA-C₁₁-BTBT-C₈**.

Synthesis of **monomers 1, 2** was carried out according to the literature methods^{4,5}. To obtain the **PMS-C₁₁-BTBT-C₈** polymer, coupling of monomer 1 to poly(methylhydrosiloxane) as a polymer analogous reaction was used in the presence of Karstedt's catalyst at 80°C (Scheme 1a). The **PMA-C₁₁-BTBT-C₈** polymer was synthesized via free-radical polymerization in dry degassed benzene in the presence of AIBN as an initiator at 80°C (Scheme 1b)⁶.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (project № 075-15-2024-560).

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Synthesis and Properties of Novel Promising Semiconducting Polymers for Organic Electronics

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The main challenge today is to design and synthesize new polymeric semiconductors that can replace classical silicon, which is approaching its physical limits. This challenge is driven by three key demands: (1) the need for energy efficient materials, (2) the transition to nanoscale organic electronic devices, and (3) the creation of flexible, wearable, and biocompatible systems. Replacing small molecule materials with polymers is a crucial step for large area inkjet printing technologies, which are increasingly important for lightweight, low cost, and flexible electronics. Polymers offer distinct advantages over small molecules in printing, including better processability, enhanced environmental stability, and potential for scalable and cost effective manufacturing. These benefits enable the formation of high quality uniform thin films over large areas, which is essential for commercial applications ¹.

This report presents the synthesis of new comb shaped polymers bearing benzothieno[3,2 b]benzothiophene (BTBT) moieties as side groups, along with a comparative analysis of their properties. The BTBT fragments impart unique electronic characteristics—extended conjugation length and improved charge transport capabilities. The innovative aspect lies in the design and synthesis of comb like architectures with pendant BTBT units, an approach that has not been extensively explored in the literature ^{2,3}. The molecular design aims to enhance both molecular ordering and π - π stacking interactions, thereby boosting charge mobility and device performance ⁴. We systematically investigated the structural features, electronic properties, and the ability of these polymers to form ordered morphologies on substrates. The highest hole mobility reached $2 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ⁵.

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

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Low-molecular semiconductors based on [1]benzothieno[3,2-b][1]benzothiophene (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 broadly studied; however, their semiconductor properties degrade significantly over time due to phase segregation in the film². A solution to this problem is incorporating BTBT fragments into the side chains or backbones of polymers.

A comparative study of conjugated polymers based on alkylthiophene-functionalized BTBT is presented. Two synthetic routes were explored: oxidative homopolymerization and Stille polycondensation. A series of polymers incorporating 0, 1, and 2 thiophene spacers was synthesized to systematically investigate the spacer length effect on the properties. The optical and electrochemical properties were characterized by UV-vis spectroscopy and cyclic voltammetry. Increasing the spacer length leads to a gradual narrowing of the optical bandgap and an increase in the HOMO level from -5.4 eV to -5.0...-5.1 eV, while the LUMO levels remain almost unchanged. All polymers exhibit p-type charge transport in organic field-effect transistors (OFETs) under ambient conditions. The highest mobility of 0.001 cm²·V⁻¹·s⁻¹ was achieved for the polymer with a bithiophene spacer. The bathochromic shift observed upon transition from solution to film is attributed to chain planarization and intermolecular aggregation.

The synthesized polymers demonstrate good stability, exhibit narrower band gaps compared to their low-molecular-weight analogues³ and high solubility in chlorine-free organic solvents, indicating their strong potential for printed electronics applications.

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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Novel Polymers with BTBT-Containing Side Chains as Semiconducting Materials for OFETs

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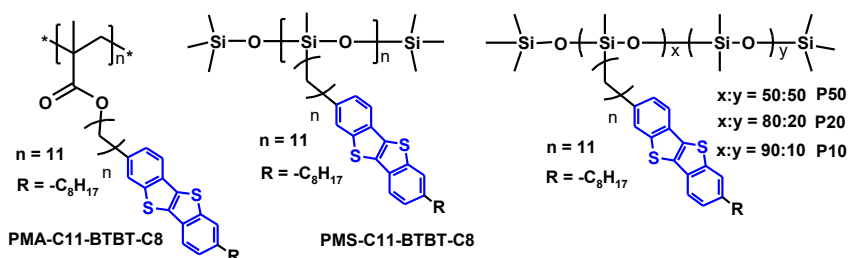
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The development of organic semiconductors (OSCs) for organic field-effect transistors (OFETs) has progressed significantly; however, the combination of high charge carriers' mobility and long-term stability remains a key challenge for widespread application. One of the most popular small-molecule OSCs is 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene (C8-BTBT). Despite the dewetting tendency of its thin films during storage,¹ this OSC is widely used owing to its proven ability to enable high-mobility electronic devices. As polymers have better processability and more stable thin film morphologies than small-molecule OSCs, several attempts have been made to create polymers with BTBT moieties. In spite of these attempts, polymers with a BTBT core in the side chains are still scarce. In this study, we investigated the electrical properties of new polymers consisting of a siloxane and methacrylate backbone with BTBT-containing side chains (Fig.1).² The best charge carrier mobility was demonstrated by a siloxane copolymer (**P50**) comprising 50% methylsiloxane units functionalized with undecyl-[1]benzothieno[3,2-b][1]benzothiophene-octyl (C11-BTBT-C6) side chains.³ To combine the advantages of polymeric and small-molecule OSCs, **P50** was mixed with the small molecule C8-BTBT to enable co-crystallization. The successful formation of co-crystalline lamellae was verified via differential scanning calorimetry and X-ray scattering, and a corresponding packing model for the BTBT units was developed. OFETs fabricated from these blends exhibited enhanced long-term stability and achieved charge carrier mobilities of up to 0.45 cm² V⁻¹s⁻¹, a value comparable to that of pure C8-BTBT devices manufactured under identical conditions.⁴



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Sensory Response Peculiarities of Organic Field-Effect Transistors

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Organic field-effect transistors (OFETs) were found to be highly sensitive to the environment air composition 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 a lack of understanding of the fundamental operation of such sensor devices.^{2,3} The researches came to the agreement only in two fundamental relations – the thinner the semiconductor layer the higher the device sensitivity⁴ and sensory response mechanism of NO₂ sensing should be related to the OFET doping.⁵ In common researches describe sensing mechanism of OFET through analyte sorption on the semiconductor surface leading to 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 talk, the sensory properties of OFETs based on various benzothienobenzothiophene derivatives will be presented and discussed. The findings demonstrated 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.⁶ 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). In addition, it was shown that in some cases (sensing NO₂ for instance) sensitivity of the devices depends on the density of free charge traps, and the higher the density of free traps, the higher the sensitivity.⁷ Also the further verification the suggested factors affecting on sensory mechanism will be presented using OFETs based on thiophene-phenylene and aryl-diazafluoren⁸ derivatives. *This work was performed under support of the Ministry of Science and Higher Education of the Russian Federation (FFSM-2025-0001).*

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Modulation of Trap Density for Low Voltage Operation in Solution Processed Organic Field Effect Transistor

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Organic field-effect transistors (OFETs) are important active components for mechanically flexible, lightweight electronic platforms, including integrated circuits, sensors, displays, and optoelectronic systems.¹ In contrast to inorganic transistors, organic semiconductors can be processed from solution on diverse substrates and are therefore attractive for large-area manufacturing, printed electronics, and wearable devices. Small-molecule benzothienobenzothiophene (BTBT) derivatives are especially attractive p-type semiconductors because the fused aromatic core promotes efficient π -stacking, high crystallinity, and favorable molecular packing. Related C₈-BTBT liquid crystalline derivatives have been widely investigated for solution-processed transistors, contact engineering, crystalline thin-film growth, and bias-stress stability.² Polymer dielectrics such as Polymethylmethacrylate (PMMA)⁴ and Polystyrene (PS) provide smooth, hydrophobic surfaces and can reduce interfacial trapping, while high-k dielectrics like Carboxymethyl cellulose (CMC), Cyanoethylated cellulose (CEC) reduce the device operating voltage required to accumulate charge carriers.³

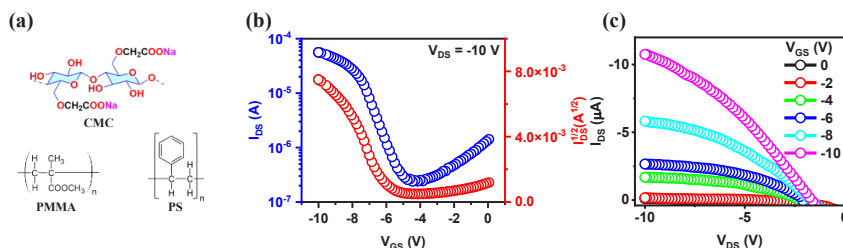


Fig 1: (a) Chemical structure of CMC, PMMA, PS; (b) Transfer and (c) Output curve of Ph-BTBT-C8 OFET on CMC-PS dielectric.

Here, we report fully solution processed C₈-Ph-BTBT OFETs using CMC-based layered dielectrics combined with PMMA, PS. Among the tested devices, CMC-PS bilayer dielectric provides the most balanced performance, with a threshold voltage of 5.96 V, subthreshold swing of 1.48 V/dec, and the lowest interface trap density of $0.90 \times 10^{12} \text{ eV}^{-1} \text{ cm}^{-2}$. The results demonstrate that coupling a biodegradable CMC layer with a hydrophobic PS interlayer is a practical route for improving dielectric-semiconductor interface quality in sustainable, low-voltage OFETs.

This work was supported by SERB grant (CRG/2022/008007), Technical Research Center second phase at IACS & DST Inspire Fellowship).

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CMC Dielectric-Based Organic Field-Effect Transistors for Low operational voltage, Flexible and Mimicking Biological Synapse

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The realization of artificial synapses using electronic devices has emerged as a fundamental strategy for neuromorphic computing and next-generation artificial neural networks. Among various approaches, Bio- inspired organic field-effect transistors (OFETs) have attracted significant attention owing to their mechanical flexibility, biocompatibility, low-cost fabrication, and compatibility with large-area printing and roll-to-roll manufacturing processes. Herein, we report a low-voltage, flexible organic field-effect transistor (OFET) employing a carboxymethyl cellulose (CMC)-based dielectric layer for the emulation of biological synaptic functions. The device exhibits controllable conductance modulation under electrical stimulation, enabling the realization of key synaptic behaviors analogous to those observed in biological neural systems.

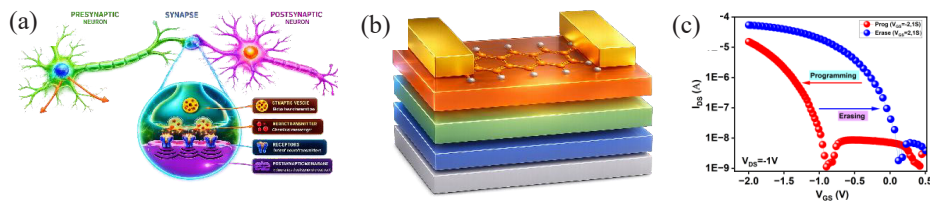


Fig. 1. (a) Biological Synapse Analogy (b) OFET Structure (c) Electrical Memory Behavior.

The fabricated OFET exhibits stable transistor operation at low operating voltages ($V_{th} = -0.70$ V) and demonstrates a good memory window of approximately 1.1 V, indicating efficient charge trapping characteristics. Synaptic functionalities were investigated using electrical pulse stimuli, where the device successfully emulated excitatory and inhibitory post-synaptic current responses. Furthermore, essential synaptic plasticity behaviors, including paired-pulse facilitation (PPF), spike-voltage-dependent plasticity (SVDP), spike-duration-dependent plasticity (SDDP), and spike-rate-dependent plasticity (SRDP), were demonstrated through systematic modulation of pulse amplitude, duration, and frequency. Continuous and reversible conductance modulation during potentiation and depression cycles further confirms the capability of the device to mimic learning and memory processes in biological neural networks. In addition, the device exhibited robust synaptic functionality even under bending conditions, highlighting its potential for flexible and wearable neuromorphic applications. These results establish CMC dielectric-based OFETs as promising candidates for low-power artificial synapses and future neuromorphic computing technologies.

This work was supported by SERB grant (CRG/2022/008007), Technical Research Center second phase at IACS).

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Direct Optical Generation of Interfacial Charge-Transfer States in Organic Donor/Acceptor Blends: What is the Difference from Exciton-Mediated Generation?

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Charge-transfer state (CTS) – coulombically bound electron-hole pair at donor/acceptor interface – is the principal intermediate of photoelectric conversion in organic solar cells and photodetectors. It is generated upon illumination of donor/acceptor bulk heterojunction (BHJ) – the common active layer material for these devices. There are two different ways of CTS photogeneration in organic donor/acceptor BHJ. The photons with sufficiently high energy (above-gap photons) are absorbed by donor or acceptor molecule, creating molecular excitons. The excitons are spitted donor/acceptor interface, producing the exciton-mediated CTSs. An alternative way of CTS generation is operative for below-gap photons. It still can be captured by BHJ blend to produce CTS directly, bypassing molecular excites states. This process is responsible for charge transfer band (CT-band) in absorption spectrum of organic BHJs, and can be utilized in organic IR-photodetectors.¹

The properties of CTS, in particular, the electron-hole distance within the CTS, significantly influence the performance of organic solar cells and photodetectors. However, the data on the CTS structure are scarce at present, and the geometry of CTS produced by direct and exciton-mediated path was not compared before. In the present work we used electron spin echo (ESE) spectroscopy to perform such comparison. For BHJ blend of donor polymer P3HT and non-fullerene acceptor IT-4F we detected ESE signal of CTS under above gap ($\lambda = 527$ nm) and below gap ($\lambda = 1064$ nm) pulse laser excitation. Analysis of out-of-phase ESE traces² allowed to reconstruct the electron-hole distribution function. Surprisingly, we found that the electron-hole distance within CTS is larger for its direct generation than for exciton-mediated generation, both for thermalized CTS and for CTS during thermalization. Presumably, this is explained by more efficient direct CTS generation in more ordered crystalline-like regions of D/A interface, while the efficiency exciton-mediated CTS generation is homogeneous over the BHJ.

Therefore, low photon energy does not necessary mean short charge thermalization length and fast geminate recombination for directly generated CTS. Instead, direct CTS generation may facilitate further CTS dissociation and photocurrent production, which can be used for design of sensitive organic IR photodetectors.

This work was supported by the RSF grant № 23-73-00072.

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Suppression of Light- and Radiation-Induced Halide Phase Segregation in CsPbI₂Br through Compositional Engineering

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All-inorganic perovskite materials, such as CsPbX₃ (X = I, Br), have attracted significant attention due to their chemical robustness and optoelectronic properties, which enable high power conversion efficiencies (PCE) in solar cells. Among them, CsPbI₂Br, obtained by partial substitution of iodide with bromide ions, is of particular interest: this material offers an optimal balance between bandgap (1.92 eV) and stability, making it promising for optoelectronic applications, including tandem solar cells. At the same time, CsPbI₂Br is prone to light-induced halide segregation, which leads to the formation of bromide-rich and iodide-rich domains and, consequently, to the degradation of photophysical properties¹. Moreover, exposure to ionizing radiation also triggers halide phase segregation, further limiting the material's stability under intense irradiation conditions.

Given the growing interest in deploying perovskite solar cells in spacecraft and other radiation-intensive environments, a comprehensive assessment of their radiation tolerance becomes a prerequisite for practical implementation. It is precisely for this reason that understanding the mechanisms of radiation-induced degradation and developing approaches for its suppression represent a key challenge toward the application of PSCs in areas where conventional silicon photovoltaics face serious weight and cost constraints. To overcome halide phase segregation, various approaches have been proposed, ranging from organic passivation or B-site compositional engineering, where Pb²⁺ is partially replaced by other metal cations².

In the present study, we have demonstrated that light-induced phase segregation can be effectively suppressed through appropriate compositional engineering. Furthermore, the developed materials and devices based thereon exhibit high radiation and thermal stability, which is a decisive factor for their operation in extreme environments—in outer space or in settings with high levels of ionizing radiation. Thus, the obtained results provide valuable insights for the targeted optimization of the performance and durability of all-inorganic perovskites for advanced optoelectronic technologies.

This work was supported by the Russian Science Foundation (project No. 22-13-00463-P).

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Optimization of Slot-Die Printing Technology of Self-Assembling Monolayers on NiOx Surface for Perovskite Solar Cells

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The use of solution-processed self-assembled monolayers (SAMs) to passivate metal oxide thin films is an effective approach for high-performance p-i-n perovskite solar cells. However, the application of SAMs in slot-die coated perovskite solar modules (PSM) is a complex technological challenge due to the strict requirements for the structure of the SAM molecule and the solvent used for printing. Commonly used SAMs suffer from poor uniformity and wettability, leading to incomplete coverage. This limits their suitability for scalable slot-die coating.

In this work, we synthesized a 4,4',4''-nitrotribenzoic acid (TPA-3C) that directly addresses the solvatophobicity and wetting mismatch of conventional carbazole-phosphonic acid SAMs under slot die processing. The three functionalities and star-shaped symmetry of the TPA-3C molecule make it possible to avoid orientation of the molecule with the non-anchoring groups toward the substrate during solution printing. We studied the data on boiling point, viscosity, solubility and the ability to form stable solvate crystals with TPA-3C of various solvents. It was determined that alcohols (ethanol, isopropanol) are the most suitable for slot-die coating of SAMs. Molecular engineering, optimal solvent selection, and coating method allow simultaneous control of wettability and surface potential, resulting in highly uniform coating of self-assembled monolayers and perovskite crystallization. In this work, we compare synthesized TPA-3C with commercial 4-(3,6-Dimethyl-9H-carbazol-9-yl)butylphosphonic acid (Me-4PACz).

One of the most important criteria for a substrate for perovskite slot-die coating is surface wettability. By investigation the wettability maps of SAMs printed on 50x50 mm² substrates, we showed that TPA3C forms a more uniform layer with a lower average water contact angle (30°) than Me-4PACz (53°). The presence of local maxima in the wettability map of a substrate with a commercial SAM led to the formation of micropores and unevenness in the thickness of the perovskite film.

We fabricated p-i-n PSCs and 12 cell modules (14.88 cm² area). We made a special focus on data fluctuations, standard deviation on recombination, transport and photoelectric performance of devices and modules. Both the Me-4PACz and TPA-3C configurations achieved efficiencies of 19 % and >1000 hours stability under ISOS-L-2 stress. However, the presence of rough spots on perovskite films crystallized on Me-4PACz leads to a wide range of values of device characteristics, carrier lifetimes extracted from TPV and TRPL, and values of external quantum efficiency. As a result, modules fabricated using the synthesized TPA-3C monolayer demonstrated a record power conversion efficiency (PCE) of 16.33% with an average value of 15.27%, while for Me-4PACz only a PCE of 15.04% was achieved with an average value of 13.05%. Thanks to its structure and optimally selected coating process, TPA-3C can be used in scalable and stable perovskite photovoltaics.

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

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Development of Materials with an Anchor Group for Defects Passivation as Interfacial Layers in Perovskite Solar Cells

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Perovskite solar cells (PSCs) are a rapidly developing technology, with efficiency increasing dramatically from 3.8% in 2009 to over 26% by 2026, allowing them to compete with and even outperform traditional silicon solar cells in laboratory settings ¹. These characteristics, combined with inexpensive materials and ergonomic manufacturing methods, have made PSCs a promising photovoltaic technology. The main challenge hindering the commercialization and scaling of PSCs is their low stability and degradation during device operation. A solution to this problem is the use of auxiliary layers in the PSC architecture, so-called interface layers based on organic semiconductor materials. The feature that allows such materials to effectively "eliminate" 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 self-assembly. However, the diversity of possible surface and bulk defects in perovskite necessitates the search for the optimal structure of self-assembling materials. An important role in these materials is played by the terminal group, which faces the perovskite layer and is responsible for specific interactions with the active layer. Moreover, 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 perovskite-based photovoltaic systems, both PSCs and perovskite solar modules (PSMs), as we have shown previously ²⁻⁵. However, the selection of structural blocks for this group, as well as the search for optimal substituents in it, currently remain an unexplored area of scientific knowledge.

In this work, a comprehensive study was conducted to identify the influence of the structure of triphenylamine-based materials with an anchor group on their properties. To this end, an effective synthetic route for a number of compounds was developed, and a range of their physicochemical properties (such as optical and electrochemical properties, thermal stability, and phase behavior) was studied. The surface properties of films formed from these materials were examined, and the influence of substituents and their donor-acceptor nature on the properties of the resulting compounds was determined. The potential for using these materials in PSCs and PSMs was assessed: all materials achieved efficiency values greater than 20% and good stability (loss of 20% of the initial efficiency after more than 1200 hours of continuous operation).

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

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Identifying Stable Perovskite Absorbers and Charge Transport Layers Under Electric Field Stress

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Operational instability of perovskite solar cells is often attributed to ion migration, but the isolated impact of the electric field separate from light and heat remains poorly understood. Here, we screen perovskite absorbers and transport layers to identify compositions that withstand pure electric field stress. Using PL microscopy, IR s-SNOM, SEM/EDX, and ToF-SIMS, we systematically compare a range of compositions and unravel the dominant aging pathways under a bias field of 1 V/ μm , comparable to fields experienced at the maximum power point.

Among single-cation perovskites, MAPbI₃ degrades rapidly via cathodic reduction of methylammonium and anodic oxidation of iodide. FAPbI₃ also shows poor stability, with void formation and massive formamidinium loss. In contrast, the double-cation formulation Cs_{0.15}FA_{0.85}PbI₃ exhibits the highest stability, retaining most organic cations and preserving PL intensity. Replacing MA with FA cations clearly improves stability in the cathodic region, making iodide oxidation the primary degradation pathway.

Interestingly, mixing three cations in Cs_{0.1}MA_{0.15}FA_{0.75}PbI₃ significantly stabilizes both MA and FA cations compared to their single-cation counterparts¹. However, these multication films still undergo field-induced phase segregation into MA-rich and FA-rich domains, though both polyiodide formation and phase segregation appear partially reversible².

For hole transport layers, we find that PTAA-based systems (bare PTAA and binary NiO_x/PTAA) outperform bare NiO_x³. The superior stability of PTAA arises from its chemical inertness toward the perovskite. In contrast, bare NiO_x triggers severe degradation via interfacial chemical interactions, leading to almost complete depletion of organic cations from the active layer and their accumulation in the PC₆₁BM electron transport layer, as revealed by ToF-SIMS. Finally, we show that for fullerene-based ETLs, the degradation rate directly correlates with film uniformity. PC₆₁BM ETLs deposited from chloroform exhibit high stability even after 1000 h under 1.2 V bias. In contrast, chlorobenzene-deposited films degrade severely. IR s-SNOM reveals PC₆₁BM aggregation in chlorobenzene-cast films, which we identify as the primary cause of poor uniformity and defects formation⁴.

Overall, our results establish the critical role of both perovskite composition and transport layer selection in determining device stability under pure electric field stress, providing a clear roadmap for more robust perovskite solar cells.

This work was supported by RSF (project № 25-23-00836).

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Electron-Vibrational Coupling in Boron-Free Multiple Resonance Fluorophores

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Narrow emission spectrum is highly desirable for organic light-emitting diodes (OLEDs) since it provides color purity required for displays. Recently, a novel class of compounds with exceptionally narrow emission spectrum — multiple resonance (MR) organic fluorophores — was suggested.¹ These compounds consist of polycyclic hydrocarbon core with electron-donating (e.g., nitrogen) and/or electron-withdrawing (e.g., boron) heteroatoms. The latter ‘orient’ electron density at frontier orbitals so that it reaches maxima at distinct atoms and form nodes at others. This yields non-bonding character to frontier orbitals, suppressing electron-vibrational coupling and narrowing the emission spectrum. However, relationships between the molecular structure and electron-vibrational coupling, which are of great demand for design of MR fluorophores with ultra-narrow emission spectra, are poorly established.

In this study, we performed theoretical investigation of electron-vibrational coupling in boron-free MR fluorophores. Specifically, we calculated the reorganization energies for hole/electron transfer and for optical excitation for various MR fluorophores, and traced the effect of changes in molecular structure on these quantities². The molecular regions that undergo significant geometrical changes as a result of charge acquisition are shown to be correlated with the patterns of frontier orbitals, which in turn depend on molecular structure. We anticipate that the revealed relationships will be useful for the design of MR fluorophores for OLEDs with ultra-narrow emission spectra.

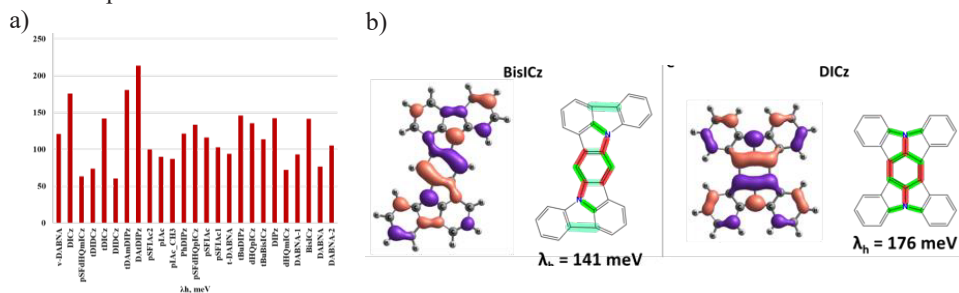


Fig. 1. Reorganization energies for hole transfer for various MR fluorophores (a). HOMO patterns and geometrical changes upon hole acquisition for two representative MR fluorophores (b). Green color depicts lengthening and red one depicts shortening; brighter color correspond to stronger changes.

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

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Blue Organic Light-Emitting Diodes Based on Novel Phenoxazine-Substituted Multiple Resonant Luminophore with Thermally Activated Delayed Fluorescence

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In the field of organic light-emitting diodes (OLED) development, the scientific community's attention is currently focused on third-generation OLEDs, which based on luminophores exhibiting the thermally activated delayed fluorescence (TADF). In TADF luminophores, the singlet and triplet levels S1 and T1 are close enough in energy that efficient thermally activated reverse intersystem crossing from the triplet state to the singlet state (T1→S1) occurs, which is where the (delayed) fluorescence (S1→S0) occurs. Therefore, both triplet and singlet excitons contribute to the EL, so the internal EL quantum yield of third-generation OLEDs can reach 100%. In 2016 a new type of so-called multiple resonant TADF luminophores was proposed.¹ These compounds are polyaromatic hydrocarbons with heteroatoms (nitrogen and boron), where the spatial separation of the frontier molecular orbitals (HOMO and LUMO), necessary for low energy differences between the S1 and T1 levels, occurs at the donor (nitrogen) and acceptor (boron) atoms. Such luminophores exhibit a narrow luminescence band (about 20–30 nm) due to their rigid molecular structure, which, in addition, minimizes nonradiative relaxation (by suppressing various types of vibrations), which ensures high photoluminescence efficiency of about 90%.¹ The most promising representative of such compounds is considered to be a molecule called DABNA (5,9-Diphenyl-5,9-diAza-13b-BoraNaphtho[3,2,1-de]Anthracene, DABNA-1), as well as its derivatives. They are promising candidates for the development of TADF materials with a pure deep blue color.

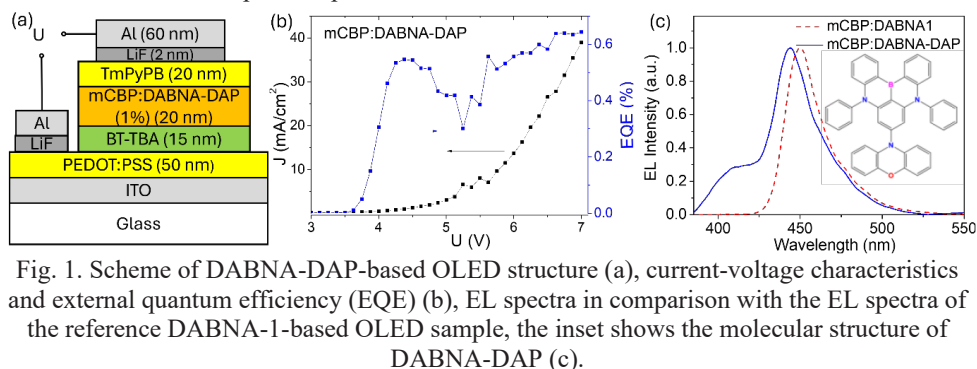


Fig. 1. Scheme of DABNA-DAP-based OLED structure (a), current-voltage characteristics and external quantum efficiency (EQE) (b), EL spectra in comparison with the EL spectra of the reference DABNA-1-based OLED sample, the inset shows the molecular structure of DABNA-DAP (c).

In the present work, we have fabricated and investigated the OLED samples based on the new phenoxazine-substituted DABNA derivative, DABNA-DAP. The device structure and its main characteristics are shown in Figure 1. Its electroluminescence (EL) provides a pure deep blue light with CIE coordinates $x=0.141$, $y=0.074$. The EL spectrum of the DABNA-DAP-based OLED (Figure 1(c), blue solid line) has a maximum at 444 nm with a FWHM of 31 nm and slightly blue-shifted relatively to the EL spectra of the reference DABNA-1-based OLED sample (Figure 1(c), red dashed line). However, in the present work, we obtain a rather low EL EQE (about 0.6%, see Figure 1(b)), which can be associated with some issues during OLED samples fabrication and characterization. Approaches for EQE enhancement are discussed. *This work was supported by the Russian Science Foundation (Project No. 24-49-02038).*

¹ Hatakeyama T., et al. *Adv. Mater.* 2016, **28**, 2777–2781.

Rational Design of Sterically Twisted D- π -A- π -D Emitters for Single-Layer OLEDs

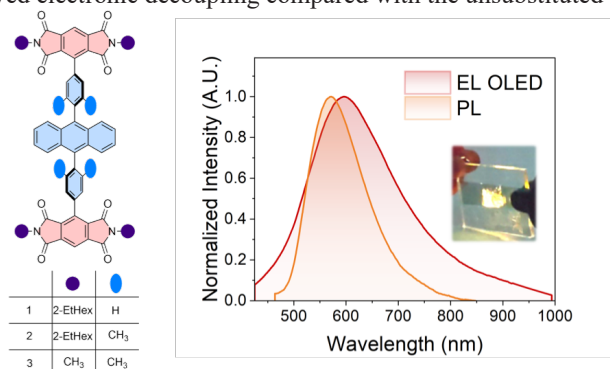
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Single-layer organic light-emitting diodes (OLEDs) have attracted considerable attention as a promising alternative to conventional multilayer OLEDs because of their simplified architecture, reduced fabrication cost, and improved manufacture. However, achieving efficient charge injection, balanced charge transport, and high electroluminescence efficiency within a single emitting layer remains a major challenge. In this work, novel donor- π -acceptor- π -donor (D- π -A- π -D) molecular architecture of OLED emitters were designed, synthesized, and comprehensively investigated for application in single-layer OLED.

The molecular design was aimed at obtaining ambipolar charge transport, a broad recombination zone, and a small singlet-triplet energy gap (ΔE_{ST}). The incorporation of a sterically hindered dimethylphenylene linker resulted in increased donor-acceptor twisting, leading to improved electronic decoupling compared with the unsubstituted analogue.



Photophysical investigations in toluene solution revealed dual fluorescence originating from locally excited (LE) and charge-transfer (CT) states. All compounds exhibited aggregation-induced emission (AIE) and crystallization-induced emission (CIE), with significantly enhanced photoluminescence quantum yields in the solid state up to 60%. Solvent-dependent fluorescence indicated the presence of twisted intramolecular charge transfer (TICT), while temperature-dependent photoluminescence measurements confirmed thermally activated delayed fluorescence. For compound **2**, an activation energy corresponding to $\Delta E_{ST} \approx 119$ meV was determined, indicating efficient reverse intersystem crossing (RISC).

Finally, compound **2** was employed as the emissive material in a prototype single-layer OLED with the structure ITO/PEDOT:PSS/2/LiF/Al. The fabricated device demonstrated electroluminescence and a low turn-on voltage of approximately 2 V, confirming the suitability of the developed molecular design for simplified OLED architectures.

These results demonstrate that rational molecular engineering of D- π -A- π -D TADF emitters provides an effective strategy for developing high-performance single-layer OLED materials and represents a promising direction for future optoelectronic applications.

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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Topological Analysis of Multi-Resonance Thermally Activated Delayed Fluorescence Materials Based on B,N-Heteroarenes for k_{RISC} and Emission Bandwidth Prediction

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MR-TADF emitters based on B,N-heteroarenes are promising OLED materials owing to their narrow emission bands and efficient delayed fluorescence. Various molecular design strategies have been employed to tune the emission wavelength, spectral width, singlet-triplet energy gap (ΔE_{ST}), and reverse intersystem crossing (k_{RISC}). [1] However, the relationship between the topology of S_1 and T_1 excited states and these photophysical parameters requires systematic quantification through hole-electron distribution analysis. [2]

We performed a topological analysis of the electronic wave functions for a series of MR-TADF compounds using Multiwfn based on the density matrices of the ground (S_0), first singlet (S_1), and triplet (T_1) excited states. A set of hole-electron descriptors was calculated and correlated with experimental emission wavelength (λ_{em}), full width at half maximum (FWHM), ΔE_{ST} , and k_{RISC} using Spearman rank analysis. Excited-state energies were obtained by DFT/TD-DFT calculations (B3LYP/6-31G(d,p)) and were further refined using a graph convolutional network (GCN) to reduce systematic prediction of S_1 and T_1 energies. Theoretical k_{RISC} values were estimated using Fermi's golden rule with spin-orbit coupling (SOC) between S_1 and T_n ($n = 1-3$). Finally, a regression model combining theoretical k_{RISC} values with topological descriptors, including the nitrogen Mayer bond order (MBO(N)), was developed.

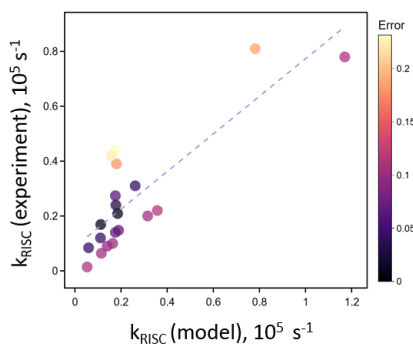


Fig. 1. Experimental vs. predicted k_{RISC} values obtained using the combined regression model (dashed line - theoretical ideal agreement; color scale - the absolute prediction error).

The combined regression model, incorporating theoretical k_{RISC} values and MBO(N), significantly improved the agreement between calculated and experimental k_{RISC} values (Fig. 1). This finding identifies nitrogen framework rigidity as a quantitative predictor of RISC efficiency and provides an efficient route for data-driven design of new MR-TADF emitters.

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

¹ *Chem. Rev.* 2024, **124**(24), 13736–14110

Universal Analytical Approach for the Transport Energy and Mobility in Disordered Organic Semiconductors

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The lack of knowledge about phonon spectra and wave functions of electron (hole) states in disordered organic semiconductors lead to the need to use some phenomenological models of hopping rates to calculate the mobility of charge carriers. The literature^{1,2,3,4} actively discusses the applicability of the common Miller-Abrahams approximation (MA), the semiclassical Marcus theory, and the so-called "empirical" model^{1,2}. The latter empirically interpolates, using the auxiliary parameter α , between the MA limit (at $\alpha = 1$) and multi-phonon quantum mechanical models^{2,3,4}. Until recently, it was believed that the transport energy concept, which provides simple analytical expressions for mobility, is applicable only in the case of the MA model.

A breakthrough in this area was a recent numerical Monte-Carlo (MC)-based study¹, which demonstrated that the transport level exists in the framework of several popular models of hopping rates. Moreover, the transport energy position is universal and does not depend on specific parameters of different hopping models.

In this paper, we demonstrated, using a modified Arkhipov method⁵, that the energy for which upward and downward jumps are equally probable is virtually independent of the hopping transition model (MA, "empirical" or Marcus) and agrees well with numerical results¹. It is precisely this energy that we identified with the transport level in our previous work (for example⁶). In agreement with numerical results of the work¹, specific parameters of a particular model (the reorganization energy in the Marcus model or the parameter α in the "empirical" model) do not significantly influence this energy.

We have derived a compact analytical expression that relates the position of the transport level to a single dimensionless parameter which combines the energetic disorder parameter and localization parameter, while in the work¹ the transport energy was presented as a color-map, where the values of these parameters were plotted along the x- and y-axes.

The universal transport energy opens the way to the simple analytical expressions for the mobility, hence for the analysis of experimental and computational data in organic photovoltaics and light-emitting devices without the need for resource-intensive numerical modeling.

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Analytic Description of Charge Carrier Mobility in Materials with Correlated Disorder Based on Modified Effective Temperature Concept

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The effect of spatial-energy correlations in disordered organic materials is the reason of so-called Poole-Frenkel field dependence of charge carrier mobility. We develop a unified analytic approach for calculating temperature and field dependence of charge carrier mobility in organic materials with correlated disorder based on modified effective temperature concept suitable for both dipole and quadrupole glasses, which utilizes previously developed approach of a carrier release from quasi-Coulomb well^{1,2}. Using the proposed model, the field dependence of mobility was calculated for different temperatures and disorder parameters (Gaussian density of states width) (Fig. 1). Calculation results show good agreement with Monte Carlo simulation data³ in the relevant field, temperature and disorder parameter range. These findings prove that modified effective temperature concept is a useful and versatile modeling tool providing simple analytic expressions for charge carrier mobility which can be used within more complicated problems.

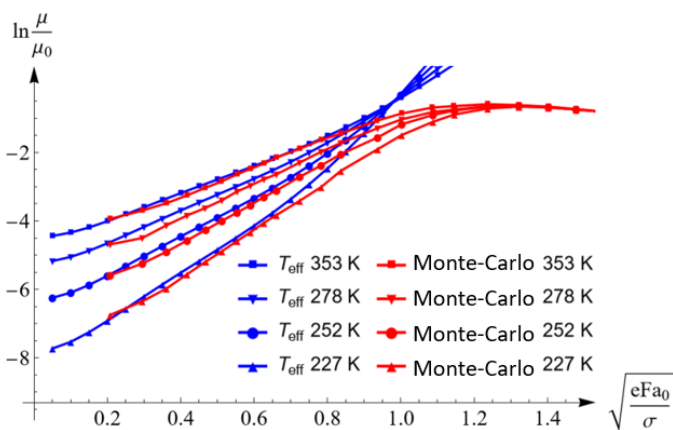


Fig. 1. Calculation results in comparison with MC simulation data³.

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Bimolecular Charge Carrier Recombination in Amorphous Semiconductors Having Spatially Correlated Exponential Density of States

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Recently it was found that the possible spatial correlation of the random energy landscape in amorphous semiconductors significantly affects the bimolecular charge carrier recombination and could lead to decrease or increase of the recombination rate constant γ depending on the nature of the disorder [1,2]. Until now this effect has been considered for the Gaussian density of states (DOS) only. In this report we consider the effect of the correlated disorder on the recombination in the exponential DOS. Correlated disorder is a common feature of amorphous organic semiconductors. At the same time, the local order in these materials could lead to the emergence of the exponential tails of the DOS [3], so the organic semiconductors could be the materials where the suggested effect takes place. Recombination in the correlated exponential DOS in the case of low temperature naturally suggest a strong dependence of the rate constant on the density of carriers n (see Fig. 1). We calculate the dependence of the recombination rate constant on temperature and density of carriers for actual examples of the random energy correlation function $c(r)$. We also consider the possibility to discriminate the suggested mechanism from other cases of the nontrivial dependence of γ on density of carriers.

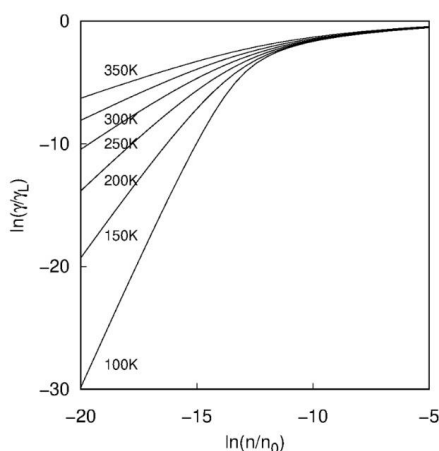


Fig. 1. Dependence of the ratio γ/γ_L on n (γ_L is the Langevin rate constant) for the exponential DOS with energy scale $E_0 = 50$ meV for different values of temperature, indicated near the corresponding curve and electrostatic dipolar disorder with $c(r) = a/r$, $a = 1$ nm, dielectric constant $\epsilon = 3$, and n_0 is the density of transport sites.

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Fine-Tuning Directional Message Passing Neural Networks: Predicting Properties of Conjugated Organic Polymers with High Accuracy

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Conjugated organic polymers are the cornerstone of modern organic photovoltaics, with wide applications as light-emitting devices, transistors, sensors, and energy-storage systems. However, their design remains difficult due to experimental synthesis and characterization being time-consuming, while accurate quantum-chemical calculations for polymeric systems are computationally demanding. In this work¹ we present a graph neural network based on the directional message-passing DimeNet++ architecture for predicting the HOMO and LUMO energy levels and the band gap of conjugated polymers directly from the three-dimensional structure of their monomers. The model was pretrained on a large dataset containing polymer-relevant TD-DFT-extrapolated electronic properties and subsequently fine-tuned on a limited dataset of experimentally measured polymer properties.

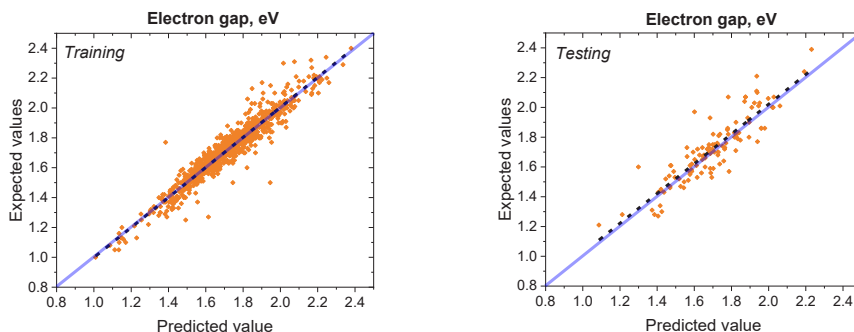


Fig. 1. Overall performance and data distribution of the pretrained model (X-axis – values, predicted by the model, Y-axis – expected values): left – electron gap on training dataset; right – electron gap on testing dataset

Direct training on the experimental data resulted in an insufficient predictive accuracy owing to the limited size of the dataset. Pretraining on single-monomer DFT data provided only limited improvement after fine-tuning, indicating that monomer-level electronic information does not adequately represent polymer behavior. In contrast, pretraining on TD-DFT data extrapolated to the polymer limit markedly improved predictive performance. The final model achieved mean absolute errors of 0.074 eV for the band gap. This result is comparable with state-of-the-art approaches² while eliminating delta-learning and time-consuming TD-DFT precomputations often utilized in similar works. The proposed framework therefore offers an efficient tool for rapid screening and targeted molecular design of conjugated polymers for organic optoelectronics.

This work was supported by RSF project (25-73-00401)

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² Liu, B., Yan, Y., Liu, M. *Nanoscale* 2025, **17**, 7865–7876

Monte Carlo Modelling of Geminate Pair Separation Probability in Disordered Organic Semiconductors

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Geminate pair separation is one of the successive steps determining the performance of organic photovoltaic devices (OPVs). Within an amorphous phase, due to the structural (off-diagonal) disorder and the energy disorder it induces, the carrier transport occurs via hopping between localized states. The permittivity of organic disordered semiconductors (ODSs) is usually small, therefore, a strongly bound geminate Coulomb pair (GP, also known as CT state) is formed after primary exciton separation. Geminate recombination limits the photogeneration yield of an OPV. Analytical description of this process is challenging. The Onsager model is still often used, despite its severe limitations: 1) it was developed for continuous media, whereas the actual system consists of discrete hopping sites; 2) it ignores energetic disorder; and 3) it neglects strongly nonequilibrium (dispersive) transport at short separation times, when hops occur predominantly downward in energy. As a result, it significantly underestimates the separation probability in the low-temperature region compared to the experimental results and kinetic Monte Carlo (kMC) simulation. The modification of the Onsager model with additional parameters has offered some improvement¹.

kMC modelling helps predict the characteristics of novel ODSs and validate analytical models. Recently, kMC has been applied to investigate the effect of Gaussian energy disorder on the photogeneration internal quantum yield² and to estimate the effect of off-diagonal disorder on charge mobility and efficiency of GP separation³.

In the present study, we use kMC to model geminate pair separation probability as a function of Gaussian disorder, temperature, applied electric field, and concentration of hopping centers. The role of variable-range hopping is investigated. We pay attention 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. It is shown, in agreement with the previous work¹, that the separation probability is much higher than predicted by the Onsager model at low temperatures for non-equilibrium GPs. However, for initially thermalized GP and weak carrier localization, the impact of long jumps from low-lying states leads to a drastic drop in the separation efficiency with decreasing temperature, to or even below the Onsager model predictions. We also vary system density together with carrier localization radius to mimic materials with partial intramolecular charge delocalization and D-A blends with small domain size. The effect of off-diagonal disorder on pair separation probability is minor in conventional systems with mean hop length ~ 1 nm, but becomes noticeable in diluted media. These findings extend our knowledge of photogeneration in organic solar cells with possible implications for active-layer optimization and synthesis of novel materials.⁴

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Poster presentations

Copper Binding, Tautomeric Equilibrium, and Thermal Dehydration in Eumelanins

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Melanins are hydration-sensitive redox-active bioorganic polymers whose transport properties are controlled by both the amount and the binding state of adsorbed water^{1,2}. Copper ions are often considered a way to increase the proton concentration in eumelanin; however, copper doping can reduce its complex conductivity³. Here we address the chemical origin of this contradiction using X-ray photoelectron spectroscopy (XPS) and temperature-dependent mid-infrared spectroscopy of synthetic eumelanin (EUM), Cu-doped eumelanin (EUM-Cu), partially decarboxylated eumelanin (EUM-D), and polydopamine (PDA).

XPS shows that copper ions strongly change the oxidized tautomeric state of eumelanin. In EUM-Cu, the O=C/O-C contribution in the O 1s spectra and the C=O/C-O contribution in the C 1s spectra increase, while the N 1s components shift toward less protonated R₂N configurations. We interpret this as Cu-induced stabilization of the quinone tautomer relative to quinone-imine and quinone-methide forms. Thus, in the dry solid matrix, copper binding is not reflected only as semiquinone formation, it also restructures the oxidized part of the polymer.

Thermal mid-IR spectra recorded after stepwise vacuum heating show that heating mainly removes water and redistributes existing functional-group contributions rather than producing new dominant absorption bands. The 3400-3700 cm⁻¹ region, assigned to weakly bound O-H vibrations, decreases almost completely by 80-100°C. In contrast, the 2400-3200 cm⁻¹ region, associated with hindered O-H stretching of strongly bound water, decreases throughout the heating series. EUM-Cu displays the largest strongly bound water contribution above 100 °C, consistent with water molecules being incorporated into the inner coordination sphere of Cu²⁺⁺ ions. At the same time, copper does not noticeably stabilize carboxyl groups against thermal decarboxylation. PDA, lacking DHICA carboxyl groups, shows the smallest spectral changes and the highest thermal stability.

These results indicate that copper ions increase the total water uptake of eumelanin through chemical binding, but part of this water is coordinatively trapped and cannot efficiently participate in a proton-transport network. Together with the immobilization of semiquinone sites in copper coordination complexes, this provides a microscopic explanation for the decrease in charge mobility in Cu-doped hydrated eumelanin.

This work was supported by the Russian Science Foundation (project No. 25-12-00134).

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2,2'-Bipyridines Functionalized with Diphenylphosphoryl Groups for Emitters Based on Transition Metal Complexes

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The design of luminescent transition metal complexes is of steady interest among researchers due to the possibility of their use in organic light-emitting diodes (OLED). The electron injection and charge transfer characteristics in phosphors used in the emission layer can be improved by introducing special functional groups. The diphenylphosphoryl group ($\text{Ph}_2\text{P}=\text{O}$) is an attractive candidate for modifying the ligand environment of the complex^{1,2,3} owing to its ability to improve electron transport properties of the luminophor.⁴

In this work, organic compounds based on 2,2'-bipyridine with diphenylphosphoryl groups in various positions were synthesized (Fig. 1). 2,2'-bipyridine is a convenient function for metal coordination, and such a design of objects is due to their further use as ligands for transition metal complexes. Based on this new family of ligands, iridium(III) and copper(I) complexes were obtained as potential candidates for use in OLED devices. These compounds were fully characterized by various physico-chemical methods of analysis. The photophysical characteristics of the obtained organic and organometallic objects were also studied.

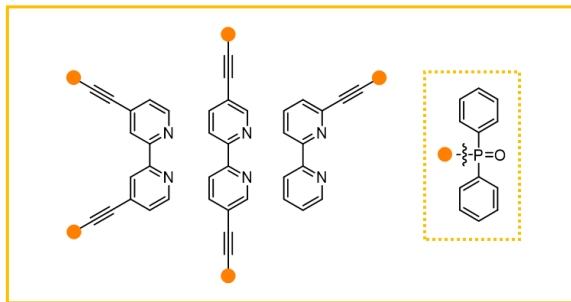


Fig. 1. Structures of the ligands synthesized in this work

This work was carried out using equipment of Research Park of St. Petersburg State University (Magnetic Resonance Research Centre, Chemical Analysis and Materials Research Centre).

This work was supported by RSF (project № 25-23-01003; design and synthesis) and was carried out within the framework of the state assignment for scientific research N 1024030700034-2-1.4.3 (photophysical investigations of 2,2'-bipyridines).

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Bis(tetracyanoselenophenoanthraquinodimethane) as Electron Acceptor for Organic Solar Cells and Photomultiplication-Type Organic Photodetectors

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Organic photodetectors are being developed to create flexible and low-cost devices as an alternative to traditional photodetectors based on inorganic semiconductors. Photomultiplication-type photodetectors are promising high-sensitivity devices in which internal gain processes allow quantum efficiency to be increased above 100%¹. The use of strong electron-deficient molecules that act as electron traps to facilitate hole injection is an advanced strategy in photomultiplication-type photodetectors design². We synthesized a molecule in which two selenophene-fused TCAQ moieties are linked by a fluorene bridge.

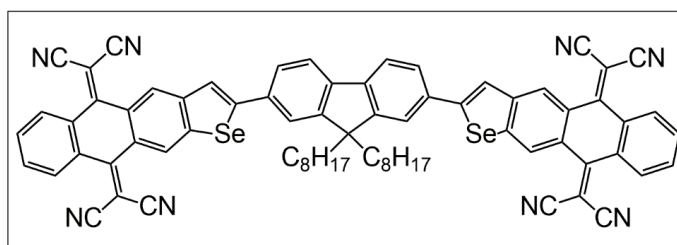


Fig. 1. Selenophene-fused TCAQ-based molecule (STCAQ)

The performance of STCAQ in solar cells similarly to thieno-fused TCAQ³. This points to low electron mobility in STCAQ, and possibility of its use in photomultiplication-type organic photodetectors, for which unbalanced electron and hole mobility is demanded. We fabricated organic photodetectors with traditional ITO/PEDOT:PSS/active layer/PFN/Field metal architecture. The active layer was PDBT-T/STCAQ BHJ. Photomultiplication under reverse bias was observed not only for low acceptor content (5%), but also for 1:1 PBDP-T/ STCAQ ratio.

This work was supported by RSF (grant № 23-73-00072).

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Tuning of Synaptic Properties by Ionogel Composition in Biocompatible Electrolyte-Gated Organic Transistors for Neuromorphic Applications

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Organic neuromorphic transistors, characterized by low power consumption, high tunability, readily available materials and low fabrication cost, present significant potential for enabling novel brain-inspired, energy-efficient and highly parallel non-von Neumann computing architectures¹.

Electrolyte-gated organic field-effect transistors (EGOFETs) based on ionogels offer long-term stability, biocompatibility and low power operation. The high capacitance of the electrolyte enables low-voltage operation and allows these devices to emulate synaptic characteristics through ion-diffusion-induced modulation of the channel potential, such as excitatory postsynaptic current (EPSC), short-term synaptic plasticity (STP), paired-pulse facilitation (PPF), and adaptation².

In this work, we investigate how the composition of a biocompatible ionogel electrolyte influences on the neuromorphic performance of P3HT-based EGOFETs. In our previous work, we demonstrated that the choice of anion effects on ionic conductivity, EDL capacitance and EDL formation time, which resulted in current decay times up to 1 s and EPSC amplitudes up to 320% with energy consumption as low as 0.1 fJ, thereby determining the speed and duration of STP signal transmission. Here, we systematically investigated the effects of anions, cations and solvent on ionogels properties and show that electrolyte composition enables precise tuning of key synaptic characteristics, including EPSC amplitude, average current decay time (τ_{avg}) and the PPF index (Fig. 1).

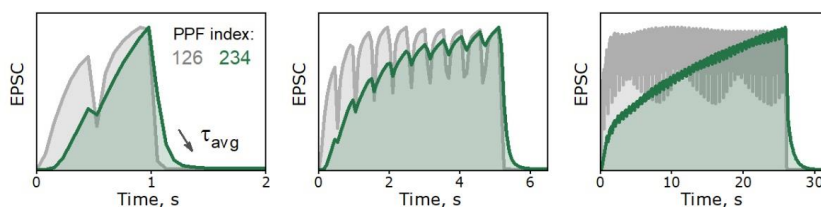


Fig. 1. Solvent effect on PPF and EPSC functions in EGOFETs.

Overall, the composition of the ionogel electrolyte plays a key role in determining the neuromorphic performance of EGOFETs. By variation the anion, cation and solvent, synaptic characteristics such as EPSC amplitude, decay time, and PPF index can be finely tuned. These results highlight ionogel structure engineering as an effective strategy for optimizing artificial synapses and neuromorphic computing devices.

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

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The Role of Ionic Migration and Cluster Formation in the Thermal Stability of CsFAPbI₃ Perovskite Solar Cells

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Thermal performance of perovskite solar cells under elevated operating temperatures remains poorly understood, being one of the key bottlenecks for commercial deployment. While composition engineering has driven record power conversion efficiencies (PCEs), its impact on defect landscape and ionic transport stability is rarely quantified at the device level under harsh thermal stress (85 °C).

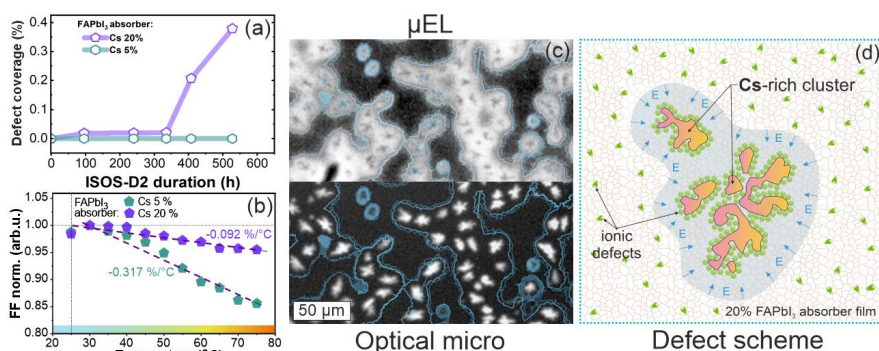


Fig. 1. Optical microscopy estimation of area covered by defects (a); Temperature dependence of FF with corresponding coefficients (b); Comparison of micro-electroluminescence and optical microscopy for Cs 20% perovskite sample after ISOS-D2 T60 (c); Scheme of Cs-rich cluster ionic defects (d).

Two Cs_xFA_{1-x}PbI₃ absorbers ($x = 0.05$ and 0.20) were compared across structural, optical and ionic transport measurements under prolonged ISOS-D-2. Devices with reduced Cs concentration achieved PCE of 22.23% with high room-temperature recombination metrics, attributed to reduced lattice strain ($\varepsilon = -0.00431$) and charge carrier lifetimes. Temperature-coefficient measurements revealed that this advantage reverses under heating, with T_{PCE} reaching $-0.624\%/^{\circ}\text{C}$ versus $-0.294\%/^{\circ}\text{C}$ for Cs 20%, driven by fill factor losses (Fig 1b). Admittance and photo-induced spectroscopies resolved an increase in ion activation energy from 0.4 to > 0.6 eV across Cs 5% and 20% compositions with different trends of diffusion coefficient. In Cs 20% devices, CsPbI₃-rich cluster formation acted as an ionic sink, passivating active interfaces (Fig. 1c, 1d), while in Cs 5% devices unimpeded ion migration along grain boundaries affected charge collection efficiency. These findings establish that room-temperature efficiency and thermal ionic stability are decoupled parameters requiring independent compositional optimization.

This work was supported by Russian Science Foundation (RSF) with grant №24-62-00022

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Synthesis and Properties of Functional Fluorescent Molecular Liquids with Trihexylsilyl Terminal Substituents

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Organic fluorescent liquids are π -conjugated luminophores with covalently attached bulky, flexible and low-melting side substituents. 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. They are already finding application in photonics and optoelectronics. Recent studies of fluorescent liquids have shown their compatibility with polymer materials, exerting not only a plasticizing effect but also changing the optical properties of the resulting composite. However, the low glass transition temperatures of molecular liquids limit their compatibility with plastics. Therefore, the development of new functional liquid materials that are not only compatible with polymers, but also participate in polymerization, is an urgent task.

In the course of this work, the series of novel liquid linear and branched luminophores containing phenylene, thiophene and benzothiadiazole units, emitting light in various ranges of the visible spectrum, were synthesized. To liquefy these oligomers the trihexylsilyl terminal substituent as most effective solubilizing group, which was identifying in our previous work¹. 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 detectors². Novel luminophores are well compatible with the polymer matrix. Based on some of these molecular liquids, liquid monomers have been obtained, the polymerization of which will make it possible to obtain new materials for optoelectronics and photonics.

This work was supported by the Russian Science Foundation (grant № 25-73-00275)

¹ Y.N. Luponosov, D.O. Balakirev, I.V. Dyadishchev, A.N. Solodukhin, M.A. Obrezkova, E.A. Svidchenko, N.M. Surin, S.A. Ponomarenko. *J. Mater. Chem. C*, 2020, **8**, 17074-17082.

² Dyadishchev, I. V., Balakirev, D. O., Kalinichenko, N. K., Svidchenko, E. A., Surin, N. M., Peregudova, S. M., Luponosov, Y. N. *Dyes and Pigments*, 2024, **224**, 112003.

Design and Photophysical Investigation of Highly Efficient Pyrene-Substituted Acridone Blue Emitters for OLED Applications

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Development of the new fully organic emitters remains one of the major challenges in organic electronics. Achieving high electroluminescence (EL) efficiency requires harvesting both singlet and triplet excitons. Two main approaches are commonly used: thermally-activated delayed fluorescence (TADF), which requires a small singlet-triplet energy gap (ΔE_{ST}), and triplet-triplet annihilation (TTA), which is feasible when the condition $2E_{T1} > E_{S1}$ is satisfied. Acridone derivatives have previously demonstrated high EL efficiency, excellent color purity, and low roll-off in OLED devices [1]. Meanwhile, pyrene derivatives are known to form excimers, exhibiting broad blue emission in the 450-470 nm region [2]. Inspired by these features, we designed three new pyrene-substituted acridone derivatives as potential deep-blue TTA-emitters.

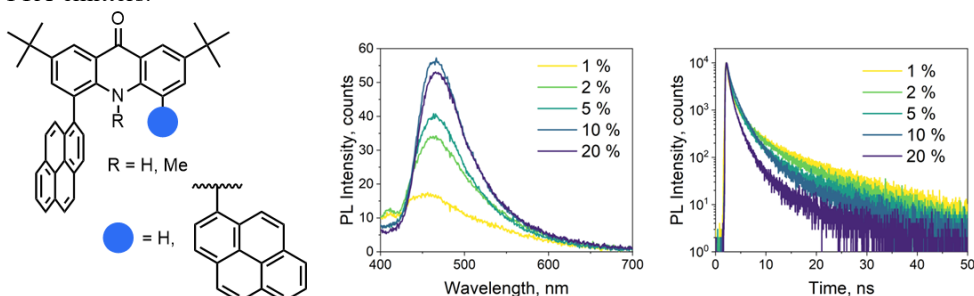


Fig. 1. Structure of studied compounds, PL and TCSPC spectra in host-guest composite with varying concentration

Density functional theory (DFT) calculations analysis predicted emission characteristics in the deep-blue spectral region. The target compounds were synthesized via three-step synthetic route involving the introducing of solubilizing substituents, bromination, and Suzuki-Miyaura coupling with pyrenyl-1-boronic acid. For methylated derivatives, an additional methylation step was performed prior to the alkylation reaction. The photophysical properties of compounds were investigated in solution, thin films, and host-guest composites.

All synthesized compounds exhibit intense blue emission with maxima at 432-441 nm and high photoluminescence quantum yield (PL QY) of 90-91% in toluene solution and 462 nm in host-guest composite. Estimated E_{S1} and E_{T1} values were found in the range 2.95-3.03 eV and 2.66-2.73 eV respectively. These results demonstrate that pyrene-substituted acridones represent promising platform for the developments of efficient blue-emitting materials and provide basis for future structural optimization.

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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²J. Wang et al. *CCS Chem.* 2021, **3**, 274–286

One-Pot Synthesis and Photophysical Properties of 4-Carboranylcoumarin Fluorophores

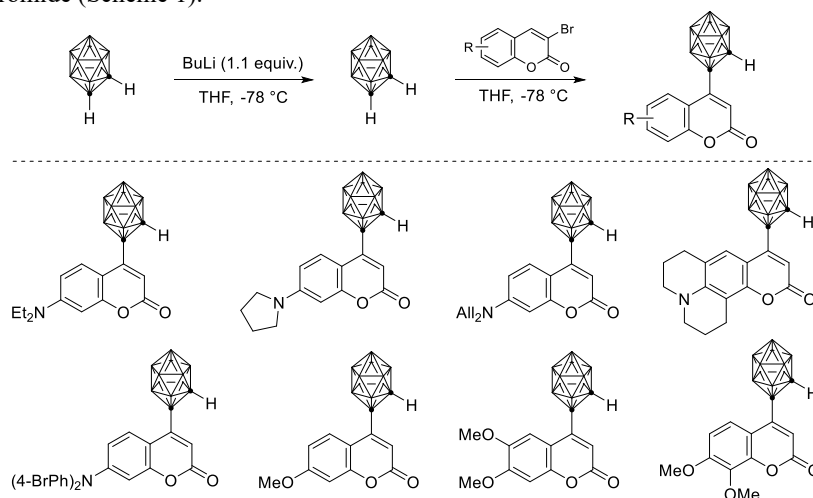
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Coumarins (2*H*-chromen-2-one), owing to their rigid, planar structure and outstanding photophysical properties, such as high fluorescence quantum yields, large Stokes shifts, and tunable emission in the visible range, represent a highly versatile and privileged scaffold for constructing functional π -conjugated small molecules that has found widespread applications in organic microelectronics. Incorporating electron-donor groups at the C7 position (typically amino or hydroxyl groups) and electron-withdrawing groups at the C3 or C4 positions creates a push-pull architecture that induces intense intramolecular charge transfer (ICT), significantly red-shifting emission and enhancing light absorption efficiency. Unlike planar organic acceptors, embedding a three-dimensional *o*-carborane core as an electron-withdrawing group can generate novel ICT pathways associated with aggregation-induced emission (AIE) or solid-state luminescence.

We found that *o*-carboranyllithium, prepared from *o*-carborane and *n*-BuLi, smoothly reacted with the corresponding 3-bromocoumarins to give 4-carboranylcoumarin fluorophores in good to high yields via a one-pot sequence of Michael addition followed by elimination of hydrobromide (Scheme 1).



Scheme 1. Synthesis of 4-carboranylcoumarins

The photophysical study demonstrated that the prepared carboranylcoumarins emitted in the visible range in solution. In addition, these fluorophores exhibited solid-state luminescence with absolute quantum yields of up to 10%.

Impact of Layers Thickness Proportion on the Charge Carrier Recombination Profile in Organic Light Emitting Diodes

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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 by charge carrier mobility, relative permittivity and mainly by energy barriers at the interface of adjacent layers. In turn, the field dependence of charge carrier mobilities leads to a change in their spatial profiles and, consequently, to the influence of layer thickness on the recombination rate profile. In this work, using drift-diffusion numerical model with direct recombination approximation and Poole-Frenkel model² of charge carrier mobility, the impact of layers thickness proportion on the charge carrier recombination profile have been investigated.

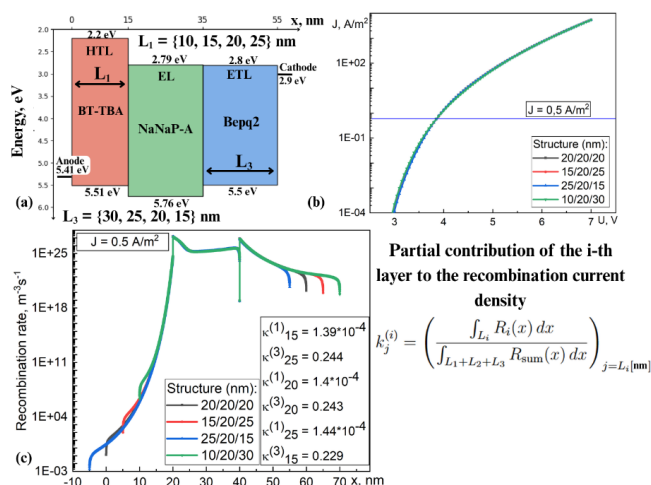


Fig. 1. OLED energy characteristics (a), current-voltage characteristics (b) and spatial distributions of the charge carrier recombination rate at current density of $J = 0.5 \text{ A/m}^2$ (c) for different combinations of transport layers thickness.

At a fixed total device thickness of 60 nm and EL thickness of 20 nm, increasing the HTL thickness from 15 to 25 nm reduces the ETL contribution to the recombination current density, with $\kappa^{(3)}$ decreasing from 0.244 to 0.229. In contrast, the HTL contribution remains nearly unchanged and negligible, $\kappa^{(1)} \approx 1.4 \times 10^{-4}$. Thus, the recombination zone can be finely adjusted by varying the relative thicknesses of the transport layers.

This work was financially supported by Ministry of Science and Higher Education, state assignment FFSM-2025-0004.

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Application of UV-Curable Siloxane Materials Bearing Covalently Bonded Luminophores as Color-Converting Layers for Blue Diodes

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Blue LEDs combined with color-converting polymer layers represent a promising route for display applications. However, conventional physical blending of luminophores into a monomer matrix suffers from aggregation and concentration quenching, which drastically reduce emission efficiency^{1,2}. In this work, a covalent immobilization strategy is proposed to solve this problem. Symmetric luminophores bearing two vinyl groups were synthesized and chemically incorporated into a siloxane oligomer backbone via UV-initiated thiol-ene photopolymerization. The vinyl groups not only anchor the dye but also act as crosslinkers, ensuring molecular-level dispersion and suppressing aggregation. The resulting UV-curable composites exhibit excellent optical transparency and intense green or red-orange photoluminescence. When coated onto a blue LED (455 nm), the siloxane layer efficiently converts the blue emission to green or orange, demonstrating the feasibility of this covalent approach for tailored light-conversion layers.

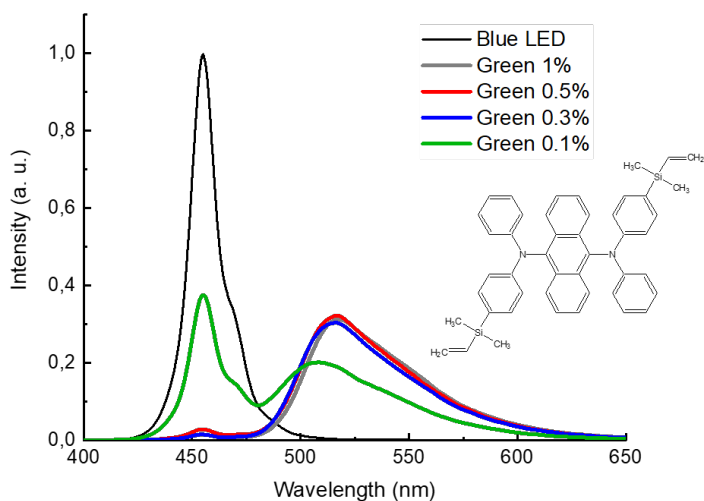


Fig. 1. Fluorescence spectra depends on the concentration of luminophor in the light-conversion layer on a blue diode

The UV-curable siloxane system allows the conversion layer to be deposited and patterned in a single photolithographic step, bypassing complex multi-stage encapsulation processes. This streamlined approach reduces the number of fabrication operations and leads to a more compact, cost-effective diode design.

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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² C. Papucci et al., *Dyes Pigments*, **188**, 109207 (2021)

Novel Triazine-Benzothiadiazole Luminophores: Design, Synthesis and Optical Characterization

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Development of new efficient organic luminophores for optoelectronic applications (OLEDs, sensors) remains a pressing challenge in modern materials science. The 1,3,5-triazine unit, owing to its pronounced electron-accepting character, serves as a versatile building block for the design of luminescent materials with tunable optical properties¹. In this work, we present the synthesis of a series of novel 2,1,3-benzothiadiazole derivatives incorporating various peripheral 1,3,5-triazine fragments. The fluorescence quantum yield reaches 78% in cyclohexane while dropping to 6% in THF, a behavior rationalized by conformational effects.

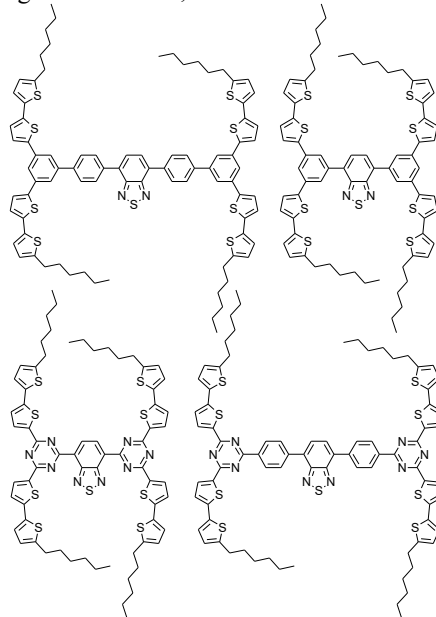


Fig. 1. Structures of the studied molecules

A comparison with recently reported meta-conjugated molecules based on 1,3,5-benzene branching centers, 2,1,3-benzothiadiazole fragments² highlights distinct structure–property relationships. In those systems, meta-connection through the 1,3,5-substituted benzene results in partial electron delocalization, and the absorption spectra can be decomposed into transitions predominantly localized on peripheral and central fragments.

Thus, the designed series of triazine-benzothiadiazole derivatives constitutes a new class of thermally stable luminophores with intense, tunable fluorescence, and represents a promising platform for active layers in organic light-emitting diodes.

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

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Charge Carrier Mobility in Organic Materials with Correlated Disorder: a Comparative Analysis of Microscopic Models and Effective Temperature Concept

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Charge carrier mobility in organic semiconductors exhibits a universal field dependence $\mu \sim \exp(F)$, which is well explained within the correlated disorder framework¹. This work presents a comparative analysis of microscopic correlation models: dipole glass (DG)¹, quadrupole glass (QG)², Gartstein–Conwell (GC) model³, and induced dipole (ID) model. The aim is to validate an analytical mobility model based on the modified effective temperature concept⁴ for different correlation types.

$$T_{eff}(T, F) = T(1 + ((\lambda e F r_0)/(kT))^n)^{1/n} \quad (1)$$

T - temperature, F - electric field strength, k - Boltzmann constant, e - elementary charge, r_0 - typical tunneling length, λ - parameter, $n = n(F, T, r_0)$.

The calculated mobility shows good agreement with Monte Carlo simulations and experimental data for polar (DEASP, DEH) and nonpolar (TPD, TASB) materials over a wide range of fields and temperatures.

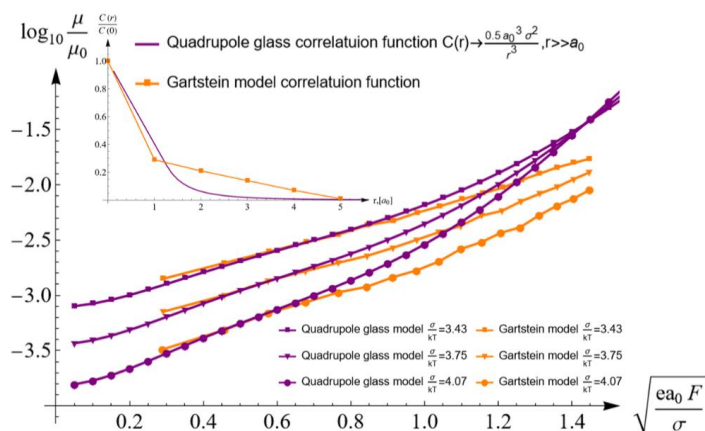


Fig. 1. Comparison of the QG and GC models. (a) Correlation functions: QG ($\sim r^{-3}$) and GC show nearly identical decay. (b) Field-dependent mobility from GC Monte Carlo simulations and QG analytical model.

The key finding is that similar correlation functions, regardless of their physical origin, yield equivalent field-dependent mobility. This is confirmed by comparing QG with GC (Fig. 1). Therefore, the shape of the correlation function, rather than its microscopic mechanism, governs charge transport. The developed model provides a simple analytical tool for mobility calculations, applicable in organic device design.

¹ Novikov S.V. *Polymer Science Series A*. 2013, **55**, 90–101.

² Saunina A. Yu., Huang L., et al. *The Journal of Physical Chemistry Letters*. 2024, **15**, 2601–2605.

³ Gartstein Yu.N., Conwell E.M. *Chemical Physics Letters*. 1995, **245**, 351–358.

⁴ Toropin A.V., Huang L., et al. *The Journal of Physical Chemistry Letters*. 2024, **15**, 3884–3892.

Conjugated Polymer Composites as Promising Hole-Transport Materials for Stable and Efficient Perovskite Solar Cells

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Perovskite solar cells (PSCs) combine high efficiency and ease of fabrication, but the main obstacles to their commercialization are related to their low operational stability. In the case of devices with n-i-p architecture the bottleneck issue is the hole transport layer (HTL) deposited atop the perovskite absorber films. Usually, it is made of heavily doped spiro-OMeTAD, which cannot provide any decent stability of PSCs. Many conjugated polymers have been evaluated as alternative HTL materials in PSCs, but their performance is usually compromised either by low hole mobility (e.g., poly(triarylamines) such as PTA or PTAA) or by poor interface contact with the surface of passivated perovskite films (vast majority of conjugated polymers).

Herein, we present a promising approach to boost the performance and stability of n-i-p PSCs by using composite HTLs. We show that composite HTL coatings enhance the stability of MAPbI₃ thin films under light exposure, and the achieved stabilization is much superior as compared to the effects provided by each of the composite components alone. Microscopy studies have revealed that composite HTLs form more uniform and compact films on the perovskite surface as compared to individual components. Due to their improved morphology, these composites exhibit good encapsulating properties and effectively block the release of gaseous photolysis byproducts from MAPbI₃, thereby enhancing perovskite thin-film stability. Furthermore, composite HTLs provide much higher photovoltaic performance as compared to the reference devices fabricated using the corresponding single-component HTLs. One composite component, which is polymer PTA, is responsible for the formation of an optimal interface with perovskite absorber films, whereas the second component facilitates charge transport to the top electrode.

Thus, the observed synergistic action of two materials combined in a composite HTL film opens a new paradigm for engineering advanced n-i-p perovskite solar cells with simultaneously enhanced efficiency and stability.

The work was supported by Ministry of Science and Higher Education of Russian Federation (project № 075-15-2024-532).

¹Komissarova E.A., Kuklin S.A., Latypova A.F., Nikitenko S.L., Ozerova V.V., Kevreva M.N., Emelianov N.A., Frolova L.A., Troshin P.A. *Mendeleev Communications*, 2024, **34**(5), 656–659.

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Study of the Influence of Deposition Parameters on the Semiconductor Properties of [1]Benzothieno[3,2-b][1]Benzothiophene Derivatives

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The continuing surge of interest in flexible and wearable electronics is further stimulating the already extensive research into organic semiconductors.

Undeniably organic semiconductors possess a number of useful properties, including flexibility, low trap density, high mobility of charge carriers and the ability to fine-tune properties via chemical modification. All of this makes this class of compounds highly promising for integration with conventional printing manufacturing technologies. Various derivatives of [1]benzothieno[3,2-b][1]benzothiophene (BTBT) are one of the most popular classes of compounds being investigated for use as active elements in organic electronics.

This work is aimed at finding optimal deposition technologies and process conditions that yield reproducible measurements of semiconductor properties. The properties of two semiconductors- poly(benzothieno[3,2-b]benzothiophene-2,7-diyl-(3,4''-dioctyl)2,2':5',2''-terthiophene-5,5'') (further P1) and 2,7-dioctyl-BTBT were investigated and compared when used in organic field-effect transistors (OFETs) fabricated with varied technological parameters (Fig. 1). The devices were prepared by four different solution-processing methods: dip-coating, spin-coating, doctor blade and drop casting. Experimental OFETs produced of C8-BTBT and P1 have shown charge carrier mobility reaching 1.8 and 0.8 cm²/Bc, respectively.

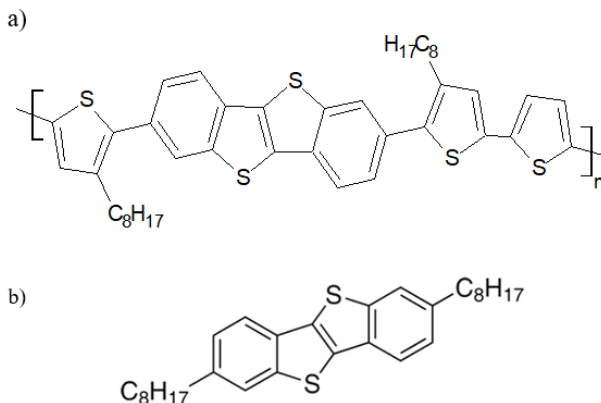


Fig. 1. The structure of a) poly(benzothieno[3,2-b]benzothiophene-2,7-diyl-(3,4''-dioctyl)2,2':5',2''-terthiophene-5,5'') and b) 2,7-dioctyl-BTBT

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).

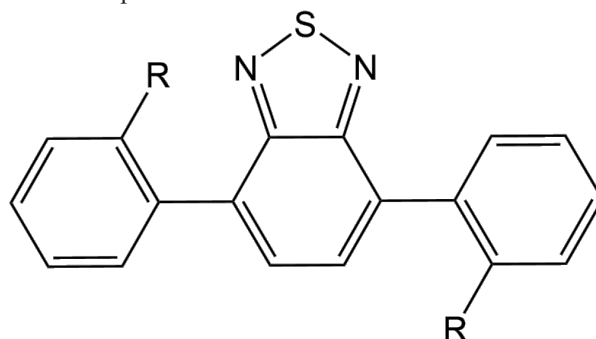
Ortho-Substituent Effects in 2,1,3-Benzothiadiazole–Phenylene Systems

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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 components¹. 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 units².



R: H, CH₃, NH₂, OH, O-CH₃, O-C₆H₁₃

Fig. 1. Chemical structure of the obtained luminophores

In this study, a synthetic approach was developed for the preparation of symmetric luminescent molecules comprising a benzothiadiazole (BTD) core as the electron-accepting component and phenyl moieties. The synthesis was accomplished via a palladium-catalyzed Suzuki cross-coupling reaction. Additionally, derivatives bearing various substituents, namely amino (–NH₂), hydroxy (–OH), methyl (–CH₃), methoxy (–OCH₃), and hexyloxy (–OC₆H₁₃) groups, were synthesized to investigate their behavior in crystalline packing. To evaluate the effect of ortho-substituents, the emission properties of these derivatives were examined in dilute tetrahydrofuran solutions, and their thermal characteristics were assessed by differential scanning calorimetry and thermogravimetric analysis.

This work was supported by RSF (project № 22-13-00255-II).

¹Skorotetsky M.S., Krivtsova E.D., Borshchev O.V., Surin N.M., Svidchenko E.A., Fedorov Y.V., Pisarev S.A., Ponomarenko S.A. *Dyes and Pigments*. 2018, **155**, 284–291.

²Stakanova D. E., Popova V. V., Svidchenko E. A., Borshchev O. V., Ponomarenko S. A. *INEOS OPEN*. 2025, **8** (1–3), 98–100.

Fabrication and Characterization of Blue OLEDs Based on Novel Multiple Resonance Diindolophenazine Derivatives

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Organic light-emitting diodes (OLEDs) represent the most successfully commercialized organic electronic devices. However, achieving blue emission with simultaneously high efficiency, color purity, and operational stability remains a significant challenge¹. Multiple resonance (MR) fluorophores have emerged as promising emitters² due to their intrinsically narrow emission spectra arising from specific patterns of frontier molecular orbitals with multiple nodes, which suppress electron-vibrational coupling. Diindolophenazine (DIPz) derivatives constitute a novel class of MR fluorophores that, when embedded in anthracene-based TTA hosts, have demonstrated ultranarrow fluorescence and reasonable OLED efficiencies. We synthesized three novel DIPz derivatives—PhDIPz, tBuPhDIPz, and MesDIPz—and fabricated OLED devices to evaluate their electroluminescent performance.

OLED displays were fabricated in the configuration shown in Figure 1a. Glass substrates with patterned ITO anodes underwent sequential cleaning in surfactant solution, distilled water rinsing, and UV/ozone treatment. PEDOT:PSS was deposited by spin-coating. All remaining organic layers and LiF/Al cathode were deposited by vacuum thermal evaporation at pressures below 5×10^{-6} mbar. Device characterization included current-voltage-luminance measurements, electroluminescence spectroscopy, and efficiency calculations using a power meter with calibrated light collection from the front surface.

The fabricated OLEDs exhibited deep-blue to sky-blue emission (fig. 1b) with maxima at 432 nm (MesDIPz), 447 nm (PhDIPz), and 453 nm (tBuPhDIPz). tBuPhDIPz-based devices demonstrated superior performance (fig. 2c) with the highest EQE (5.0%), current efficiency (2.85 cd/A), power efficiency (4.25 lm/W), and maximum luminance (16,800 cd/m² at 793 mA/cm²). These results demonstrate that rational substituent engineering of DIPz derivatives enables efficient deep-blue OLEDs with promising characteristics.

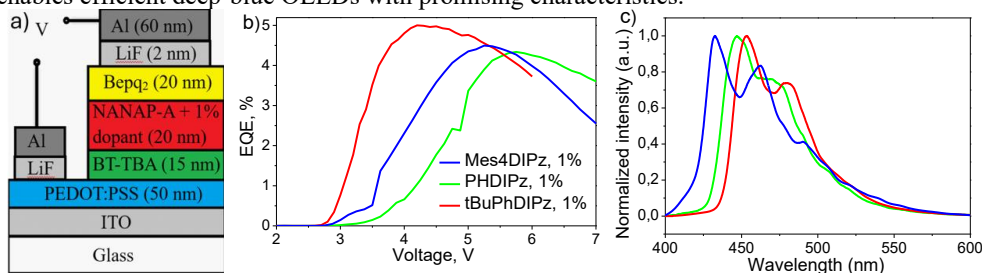


Fig. 1. OLED data for the three dopants investigated. Device schematics (a), EQE as a function of voltage (b), EL spectra (c)

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

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2. Kondo Y.Y., et al. *Nature Photonics*. 2019, **13**, 678–682.

Volatile Additive for Morphology Modification of Acceptors in the Active Layer of Organic Solar Cells

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² Novosibirsk State University

Today, organic photovoltaics is a promising and rapidly developing field of renewable energy. The key materials responsible for light absorption, charge generation, and charge transport to the electrodes within the device are organic semiconductors. Organic semiconductor materials possess a number of unique properties, including light weight, flexibility, environmental friendliness, biodegradability, and relatively low production costs¹. One of the main challenges in organic photovoltaics currently is the instability and poor controllability of the donor–acceptor composite. The morphology of the active layer can be improved by introducing substances with specific properties (volatile and non-volatile additives).

Volatile additives are compounds introduced into the solution during film formation and completely removed from the active layer during spin-coating or thermal annealing steps. In this work, the volatile additives 2-(2-methylphenyl)benzo[b]thiophene (MPBT) and 2-(2-(trifluoromethyl)phenyl)benzo[b]thiophene (TFBT) were used to improve the morphology of the PM6:Y6 composite, owing to their high solubility in organic solvents and low boiling points. Organic photovoltaic cells based on the PM6:Y6 composite with MPBT additive at various concentrations relative to the solvent mass, as well as based on the pristine composite, were fabricated and tested. For the active layer deposited from chlorobenzene, the optimal additive concentration was found to be about 5 wt.% relative to the solvent. This led to a decrease in short-circuit current and fill factor, while the overall power conversion efficiency (PCE) increased compared to the additive-free active layer².

Analysis of the additive properties showed that MPBT preferentially interacts with the acceptor component Y6. X-ray diffraction and AFM revealed significant changes in the molecular ordering of Y6 and in the film morphology upon MPBT evaporation. The selective action of the volatile additive on one of the composite components can be used for fine-tuning the active layer morphology and deliberately modifying its properties. This approach may be useful not only for the PM6:Y6 active layer but also for other donor–acceptor blends with non-fullerene acceptors. The TFBT additive was also tested for the PM6:Y6 system deposited from ortho-xylene. O-xylene, being a “green” solvent, is halogen-free, has low toxicity, and is relatively inexpensive, making it suitable for large-scale application. The introduction of the volatile TFBT additive into the active layer increased the PCE from 1% (devices based on the pristine composite) to 5% (devices with 5 wt.% TFBT relative to the solvent).

The results obtained so far demonstrate that the use of volatile additives is an effective tool for controlling the active layer morphology and improving the performance of organic solar cells. *This work was supported by the RSF. (RSF № 23-73-00072).*

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² Baranov D. S. et al. *Organic Electronics*, 2025, **144**, 10728.

EGOFET Multi-Sensor Device Design for Metal Detection in Aqueous Solutions

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The creation of a sensor device capable of quick and accurate detection of several vital metal ions in aqueous solutions simultaneously can be potentially extremely useful in many areas: from point-of-care medicine for monitoring vital parameters of a patient to environmental monitoring of water resources¹.

In this work, we set out to create a promising multisensor for detecting several metal ions based on electrolyte-gated organic field-effect transistor (EGOFET). The „multi” properties of the device are achieved due to the location of two receptor layers with two different [1]benzothiophene[3,2-b]benzothiophene (BTBT) derivatives on one wafer. The molecular composition of the combined receptor layer of multisensor device is shown on the figure 1, such chemical structure of derivatives allows both of them to apply to the substrate by Langmuir-Schaeffer technique. A molecule of functional 4,13-diaza-18-crown-6 ether attached to the semiconductor core of [1]benzothiophene[3,2-b]benzothiophene (BTBT) via an alkyl bridge was specially synthesized (Fig. 1). This crown derivative is structurally similar to the previously obtained molecule² of the BTBT siloxane dimer (D2-C7-BTBT-C6), which should improve their co-crystallization and increase the electrical properties of the receptor layer. The receptor layer with Und-BTBT-Hex-Biotin has already proven itself well³ for silver detection by aptamer functionalization. Here we use aptamers specific to mercury and lead ions, whereas the crown-ether functionalized part of the wafer is capable to detect the whole concentration of metal ions.

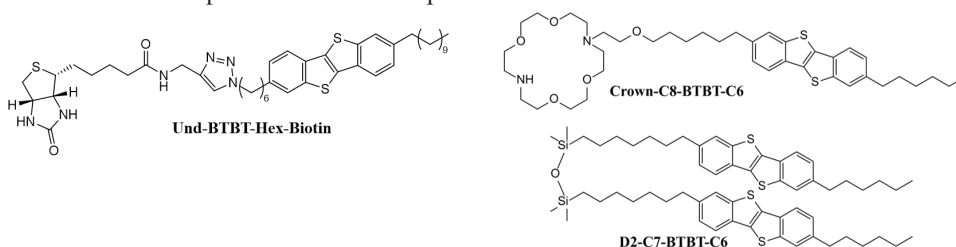


Fig. 1. Molecular composition of the combined receptor layer of multisensor device.

As a result of this work, the EGOFET device has been created capable of detection different metal ions by using selective receptor layers based on crown-ether and biotin derivatives of BTBT.

This work was supported by Russian Science Foundation (project № 23-73-00103).

¹ Shimizu F. M., Braunger M. L., Riul Jr A. *Chemosensors*. 2019, 7(3), p.36. doi:10.3390/chemosensors7030036

² Trul A.A., Chekusova V.P., Anisimov D.S., et al. *Adv Electron Mater.* 2022, 8(5), p. 2101039. doi:10.1002/aelm.202101039

³ E.Y. Poimanova et al. *J. Mater. Chem. B*, 2026, 14(8), p.2543 doi:10.1039/d5tb02347e

MR-TADF Emitters Based on Quinolino[3,2,1-*de*]Acridine-5,9-Dione (QAO)

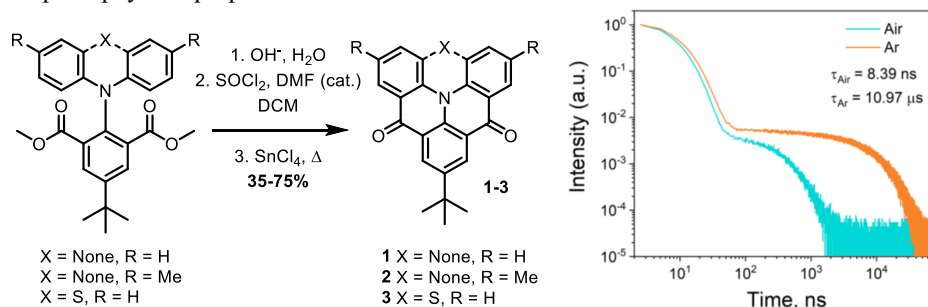
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Multi-resonance thermally-activated delayed fluorescence (MR-TADF) has emerged as one of the most effective strategies for realizing highly efficient narrowband organic emitters. In MR-TADF molecules, electron-rich and electron-deficient regions are embedded within the rigid fused aromatic framework, leading to the spatial separation of the frontier molecular orbitals. This unique electronic structure combines high oscillator strength, small singlet-triplet energy gap, thereby enabling efficient TADF with excellent color purity[1].

Herein, we report a versatile synthetic strategy for quinolino[3,2,1-*de*]acridine-5,9-diones **1-3** (QAO). The target compounds were synthesized through Ullmann C-N cross-coupling followed by intramolecular cyclization via electrophilic aromatic substitution. This approach provided efficient access to QAO-based TADF emitters (**1-3**) in good yields and enabled fine tuning of their photophysical properties.



Detailed photophysical studies revealed that incorporation of a sulfur atom into QAO framework induces a bathochromic shift of the emission spectra and enhances TADF properties. Remarkably, compound **3** exhibits TADF even in non-degassed toluene solution, indicating highly efficient reverse intersystem crossing (RISC). In degassed toluene, prompt and delayed fluorescence lifetimes measured at 8.39 ns and 10.97 μs, respectively, were obtained. In 1-wt% mCP-doped films, the delayed lifetime increased to 35.8 μs, while the photoluminescence quantum yield reached 60%.

The methyl-substituted QAO derivative (**2**) exhibits narrowband blue emission with a full width at half maximum (FWHM) of only 26 nm together with prompt and delayed fluorescence lifetimes at 8.83 ns and 3.08 μs, respectively, in degassed toluene solution. The combination of narrow emission, efficient delayed fluorescence, and high photoluminescence efficiency demonstrates that QAO-based MR-TADF emitters represent a promising platform for the development next-generation high-color purity OLED materials.

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

¹Wu X. et al. *Chem. Rev. American Chemical Society (ACS)*, 2025. Vol. **125**, № 14. P. 6685–6752.

Cationic Iridium Complexes with Carboranyl-Derived Ligands for OLED Applications

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The development of iridium complex-based organic light-emitting diodes (OLEDs) is undoubtedly a highly relevant area of modern optoelectronics due to their outstanding electroluminescent performance and nearly 100% internal quantum efficiency. The photophysical properties of these systems are largely governed by the nature of the coordinated ligands, making the design and synthesis of novel ligand architectures an important research objective. In particular, the introduction of an *ortho*-carborane moiety enables precise tuning of the electronic and steric properties of the ligand while improving the thermal and chemical stability of the resulting complexes and suppressing concentration quenching. Consequently, carborane-containing iridium complexes represent promising emitters for the development of highly efficient OLED devices.

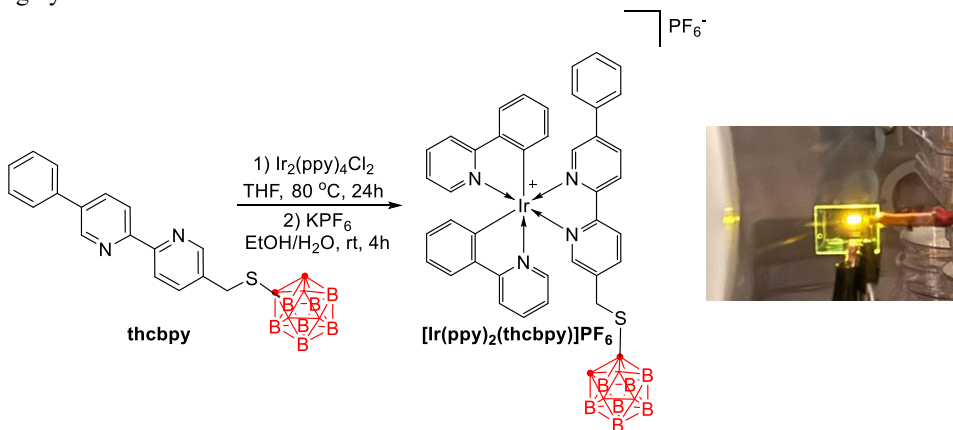


Fig. 1. Synthesis of Cationic Iridium Complexes with Carboranyl-Derived Ligands and Fabrication of an OLED

In this work, cationic iridium(III) complexes were synthesized via the reaction of *ortho*-carboranyl bipyridine ligand systems with dichlorotetrakis(2-phenylpyridine)diiridium(III). Based on one of the synthesized complexes, a prototype yellow OLED was fabricated, exhibiting a maximum luminance of 3500 cd/m².

Superior Impact Resistance in Bionic Nanocellulose Composite Supramolecular Elastomers via Multiple Hydrogen Bonding Interactions

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Impact loads under extreme conditions pose serious threats to personnel and equipment, driving the urgent need for impact-resistant materials that combine high strength and toughness. Inspired by the hierarchical structures of biological materials, this study proposes a novel biomimetic design strategy for impact-resistant elastomers. By employing supramolecular chemistry, nanocellulose and linear polyurethane molecular chains are simultaneously tailored and expanded to construct high-performance composites through multiple hydrogen bonding interactions.

In this work, 2-ureido-4[1H]-pyrimidinone (UPy), which contains quadruple hydrogen bonds, was used as a chain extender for polyurethane prepolymers and simultaneously employed to modify cellulose nanofibers (CNF). This approach established a hierarchical hydrogen bonding network between the matrix and the filler, effectively inhibiting excessive crystallization of the polycaprolactone (PCL) soft segments and promoting uniformly distributed microphase separation. At an optimal UPy-CNF loading of 0.5 wt%, the resulting composite elastomer (SPU-CNF-0.5) achieved a remarkable fracture strength of 47.5 MPa and an exceptional elongation at break of 974.2%, representing a 121% increase in strength compared to the neat SPU elastomer. Low-field NMR and variable-temperature FTIR analyses confirmed the presence of multiple hydrogen bonds (urethane double hydrogen bonds, carboxyl double hydrogen bonds, and UPy quadruple hydrogen bonds) and their reversible dissociation and reassociation under mechanical stress, which are key to the material's high energy dissipation and self-reinforcement capabilities.

In summary, through the synergistic combination of rigid nanocellulose reinforcement and dynamic UPy supramolecular networks, this study successfully developed a biomimetic elastomer integrating high strength, high toughness, and superior impact resistance, offering a promising strategy for advanced protective materials.

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Synthesis of Diindolophenazine Derivatives, Expansion of the Range of Fluorophores for the Creation of Blue OSDs

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Organic light-emitting diodes (OLEDs) are a key technology for modern displays and lighting systems due to their high efficiency, ultra-thinness, lightweightness, flexibility, and multicolor emission. The creation of reliable blue OLEDs with high efficiency and stability remains a pressing challenge, as their performance is significantly inferior to that of their green and red counterparts.

We previously reported the preparation of a new fluorophore—a diindolophenazine derivative with phenyl substituents—and the fabrication of an OLED based on it, characterized by stability, a long lifetime, and deep blue emission¹. In this study, we developed new synthetic routes and expanded the range of new fluorophores based on the diindolophenazine core. Specifically, we synthesized symmetrical 2,5,10,13-tetramesitylene-substituted, unsymmetrical 2,10-dimesitylene-substituted, and unsubstituted diindolophenazines (Fig. 1).

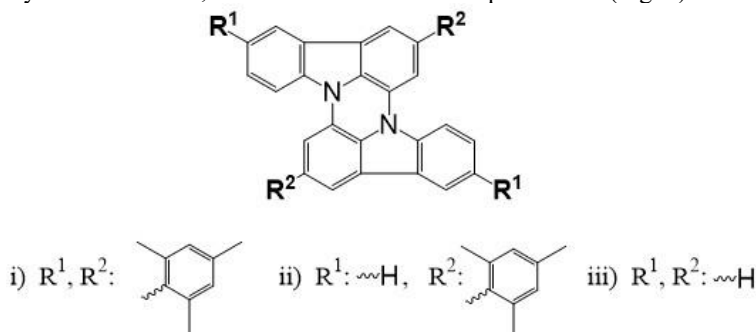


Fig. 1. Structures of the obtained fluorophores based on diindolophenazine

This work was supported by FFSM-2025-0004.

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Carbon-Based Additives for Modifying the Active Layer and Electrode Interfaces in Organic Solar Cells

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Organic photovoltaics has emerged as a promising alternative to conventional inorganic solar cells due to its unique advantages, including light weight, mechanical flexibility, solution processability, and potential for low-cost manufacturing. One of the key challenges remains the precise control over the nanoscale morphology of the bulk heterojunction active layer, which directly governs exciton dissociation, charge transport, and recombination losses. Additionally, the quality of charge-extracting interfaces, particularly the hole-transporting layer and its contact with the active layer, plays a critical role in determining device performance and stability. Among various strategies explored to address these issues, the incorporation of carbon based nanomaterials such as carbon nanotubes, graphene derivatives, and nanodiamonds - has attracted considerable interest. These materials can modify the active layer morphology, enhance charge carrier mobility, and passivate trap states. In this work, two independent approaches to improve the performance of organic solar cells based on the P3HT:PC₇₀BM donor-acceptor blend were investigated using carbon nanomaterials.

In the first approach, detonation nanodiamonds (NDs) were introduced directly into the active layer at various concentrations (1, 2.5, and 5 wt.%). A pronounced non-monotonic concentration dependence was observed: at 5 wt.%, severe aggregation of NDs disrupts the donor-acceptor network, leading to drop in photocurrent, while at 2.5 wt.%, the PCE increases from 1.01% to 1.80% and the fill factor nearly doubles (from 16.6% to 31.4%). The optimal concentration improves phase separation and reduces recombination losses. In the second approach, an interpenetrating electrode (IE) consisting of hybrids of carboxylated multi-walled carbon nanotubes with PEDOT:PSS was deposited onto the conventional PEDOT:PSS hole-transporting layer. Deposition of this electrode from water solution with concentration of 0.5 mg/ml leads to a noticeable improvement in all photovoltaic parameters. The addition of 0.05% cetyltrimethylammonium bromide (CTAB) to the hybrid dispersion further enhances dispersion quality and coating uniformity, increasing the PCE nearly fourfold (to 3.43% vs. 0.87% for reference devices) and doubling the fill factor. It is important to note that previous work¹ has shown that adding MWCNTs directly into the active layer can lead to shunting, which deteriorates OSC performance. However, insulating the MWCNTs with a polymer can prevent shunting and even improve the photovoltaic parameters. Cells incorporating IE exhibit no drop in open-circuit voltage, confirming the successful insulation of the metallic nanotube shells and the suppression of shunting paths through the PEDOT:PSS coating.

Drift-diffusion numerical modelling revealed that both approaches lead to a reduction in the bimolecular recombination constant and changes in effective carrier mobility, with suggested mechanisms: NDs act as passivators of recombination centers, while IE electrode provides percolation pathways for rapid charge collection, locally alters the morphology of the donor-acceptor blend, potentially creating P3HT domains which envelope MWCNTs.

This work was supported by the Russian Science Foundation (grant No. 23-73-00072).

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Synthesis of Bipyridine Ligand Systems Containing Thiocarborane Species

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The development of synthetic approaches to *ortho*-carborane-based ligand systems is driven by the unique chemical and physical properties of this cluster. Introduction of the carborane moiety into the ligand framework enables fine tuning of its electronic and steric properties while enhancing the thermal and chemical stability of the resulting complexes. These features make carborane-containing ligands promising building blocks for the design of catalysts, functional materials, and coordination compounds with tailored properties.

In this work, a series of *ortho*-carboranyl ligand systems was synthesized via a five-step synthetic route. The first stage involved the condensation of a hydrazone oxime with pyridine-carboxaldehyde. The resulting intermediate underwent an aza-Diels–Alder reaction followed by reduction of the carbonyl group. At the subsequent stage, a Finkelstein reaction afforded the corresponding halide derivative, which subsequently underwent nucleophilic substitution with *ortho*-mercaptocarborane to yield the target ligand systems.

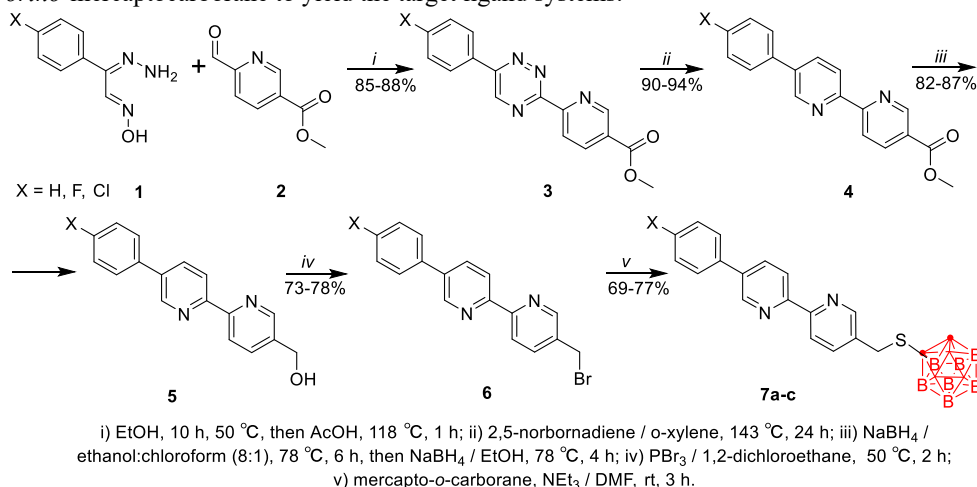


Fig. 1. Synthesis of ligands based on *ortho*-carboranyl derivatives

The synthesized compounds may serve as promising precursors for the rational design of organic luminophores and organometallic complexes intended for application in organic light-emitting diodes (OLEDs).

Copolymer Structure Determination of Carbazole- and Triazine-Containing Styrene Monomers through Copolymerization Kinetic Study Analysis

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The host–dopant approach is widely employed in OLED emissive layers. The local environment of the emitter strongly influences its photophysical properties and can either enhance or completely quench the emission¹. Although this phenomenon has been extensively investigated for small-molecule thermally activated delayed fluorescence (TADF) emitters, considerably less attention has been paid to TADF copolymers. In particular, the effect of copolymer composition remains largely unexplored, despite the substantial differences in the electronic properties of the comonomers, which may significantly alter the local environment of the emissive units and, consequently, their luminescence characteristics.

In this work, the copolymerization kinetics of donor monomers based on *N*-phenylcarbazole and 3,6-di-*tert*-butyl-*N*-phenylcarbazole with the acceptor monomer 2,4,6-triphenyl-1,3,5-triazine were investigated (Fig. 1). Homopolymers and donor–acceptor copolymers with donor-to-acceptor (D:A) ratios of 50:50, 90:10, 95:5, and 99:1 were synthesized and characterized by GPC, HPLC, ¹H and ¹³C NMR spectroscopy, elemental analysis, TGA, DSC, and optical spectroscopy of dilute THF solutions.

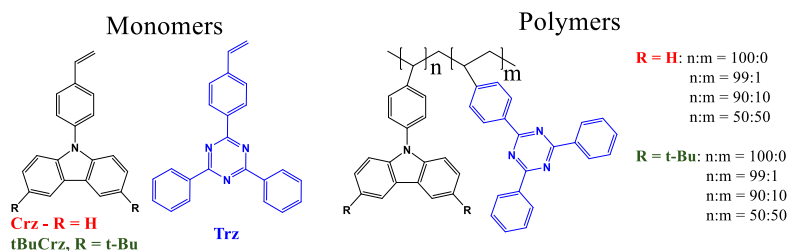


Fig. 1. Chemical structure of monomers and polymers.

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

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Synthesis and Characterization of a Series of Alkynylphosphine Sulfide Ligands

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Despite the long-standing knowledge of the phosphine sulfide moiety, its behavior within more elaborate molecular architectures remains considerably less explored than that of analogous phosphine oxides¹ and phosphonium salts². When attached to a donor fragment—for instance, an alkynyl group coordinated to a transition metal—the phosphine sulfide functionality can impart novel properties to the metal complex. In particular, the presence of the sulfur atom enables additional metal coordination, while the overall molecular motif renders these compounds promising candidates for application as surfactants in gold plasmonic nanoparticle systems³.

Furthermore, phosphine sulfides are widely employed as host materials in organic light-emitting diodes (OLEDs), owing to their favorable S– π interactions and superior charge-transport characteristics relative to their phosphine oxide counterparts⁴. Given all the properties mentioned above modified phosphine sulfides are promising ligands for luminescent metal complexes, which could be further suitable for usage as emissive dopants in OLED devices.

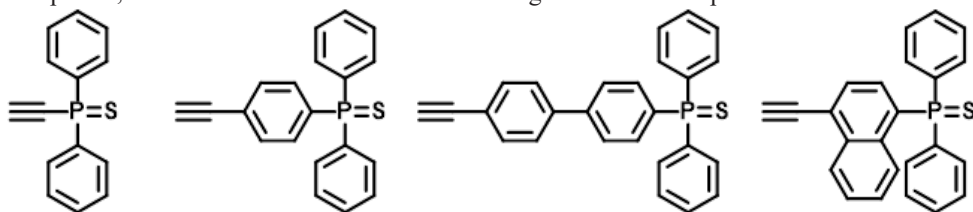


Fig. 1. Structures of the obtained compounds

In this work, a series of four alkynylphosphine sulfide ligands bearing distinct aromatic linkers between the donor site and the phosphine sulfide group was synthesized and fully characterized. Notably, the resulting compounds display only weak emission in the crystalline state, yet they become luminescent upon melting into a glassy form.

This work was carried out using equipment from the Resource Centers of the St. Petersburg State University Research Park: "Magnetic Resonance Research Methods", "Methods of Material Composition Analysis", "X-ray Diffraction Methods for Material Research" and the "Cryogenic Department."

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³ Chung W., Simmonds A., Griebel J., Kim E., Sug H. *Angew. Chem. Int. Ed.*, 2011, **50**, 11409–11412.

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Controlled Architecture of BTBT-Grafted Copolymers via Wittig, Hydrosilylation, and Click Chemistry: Towards Functional Receptor Layers

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Organic bioelectronic devices, particularly electrolyte-gated organic field-effect transistors (EGOFETs), demand receptor layers that combine high charge-carrier mobility with specific biorecognition ability. The [1]benzothieno[3,2-b][1]benzothiophene (BTBT) core is widely recognized for its excellent self-organization and transport properties, whereas biotin provides a universal anchor for streptavidin-based immobilisation of various bioreceptors. However, the integration of both moieties into a single polymer matrix with controlled architecture remains a challenging task¹.

In this work, we report two complementary synthetic strategies yielding novel copolymers with grafted BTBTⁱⁱ and biotin side groups. The first and main approach focuses on styrene-based copolymers. The synthesis begins with a Wittig reaction to introduce the BTBT-containing substituent into a styrenic monomer, followed by radical copolymerisation with styrene to afford a polymer backbone with pendant BTBT units. Subsequently, the biotin moiety is attached via an azide–alkyne cycloaddition (click reaction) to alkyne-functionalised comonomer units pre-introduced in the copolymer. This sequence (Wittig → copolymerisation → click) provides precise control over the BTBT/biotin ratio and yields processable materials with good film-forming properties.

The second route involves siloxane-based copolymers prepared by polymer-analogous transformations of a poly(methylhydride-dimethyl)siloxane backbone. Here, BTBT groups are grafted via hydrosilylation, then the remaining groups are converted through Williamson etherification, and finally biotin is attached by a separate azide–alkyne cycloaddition. Both families of copolymers were thoroughly characterised with respect to phase behaviour, thermal stability, and self-assembly.

Langmuir–Schaefer technique demonstrated pronounced self-organisation of the copolymers at the air–water interface, allowing the formation of highly ordered receptor layers. The polymeric nature of the receptor layer substantially improved the reproducibility of measurements, which is a critical advantage for practical biosensing. Among the two types, the styrene-based copolymers showed fine film uniformity and easier processing, making them particularly attractive for large-area sensor arrays.

Overall, specifically the developed styrene-based copolymers represent a versatile platform for the fabrication of highly sensitive and reproducible EGOFET biosensors.

This work was carried out with the support of the Russian Ministry of Science and Higher Education (topic FFSM-2024-0003)

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Organic Photosensitizers Based on Indolo[3,2-*b*]carbazole with an A- π -D- π -A Structure for Dye-Sensitized Solar Cells

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The quest for photovoltaic technologies that harmonize high efficiency with low cost and sustainable materials has been a central driving force in the evolution of third-generation solar cells. Among these, dye-sensitized solar cells (DSSCs) have emerged as a particularly promising candidate, renowned for their potential for low-cost fabrication and remarkable performance under both ambient and indoor lighting conditions ¹.

The general principle of DSSCs operation is based on a light absorption with dye-sensitizer, excitation and charge separation, followed by injection of an excited photoelectron into the conduction band of nanocrystalline TiO₂ ². Therefore, the dye plays a key role in a device performance.

Metal-free organic dyes have several advantages in comparison with Ru(II)-based dyes and metal-porphyrin complexes to use in DSSCs, like high molar extinction coefficients, tunable optical and electrochemical properties, low cost of their synthesis due to the use of easy-to-follow procedures, and inexpensive chemicals. In general, the most effective organic dyes contain at least a donor (D) and acceptor (A) unit linked through a π -linker.

The donor part plays a pivotal role in this system. In this regard, 5,11-Dihydroindolo[3,2-*b*]carbazole (indolo[3,2-*b*]carbazole, ICZ) has attracted increasing attention as a donor building block for organic optoelectronic materials and DSSC sensitizers³. Structurally, ICZ can be viewed as a ladder-type π -system formed by fusion of an indole unit with a carbazole core. This fusion significantly extends the π -conjugated system relative to carbazole, increasing electron density and enhancing the electron-donating strength of the core.

Herein, we report the synthesis of dyes with an A- π -D- π -A structure containing an indolo[3,2-*b*]carbazole fragment as the electron-donating moiety. Their physicochemical and photovoltaic properties were investigated. For the most efficient compounds, the temperature dependence of their photovoltaic performance was additionally examined.

This work was supported by Russian Science Foundation (project № 25-23-01204, <https://rscf.ru/en/project/25-23-01204/>).

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Semiconductor Properties of Novel Highly Soluble 2,7-diphenyl-[1]benzothieno[3,2-b][1]benzothiophene Derivative in Organic Field Effect Transistors

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Derivatives of [1]benzothieno[3,2-b][1]benzothiophene (BTBT) are one of the most promising classes organic semiconductors used as active elements in organic electronics, in particular in organic field effect transistors (OFETs). Due to the high chemical and thermal stability of the BTBT fragment, structural modification is possible by introducing conjugated substituents and solubilizing groups, which contributes to the orderly self-organization of semiconductor molecules and the formation of crystal lattices.

In this work, the semiconductor properties of a novel highly soluble derivative of BTBT – 2,7-bis(4-ethylhexylphenyl)[1]benzothieno[3,2-b][1]benzothiophene (EH-P-BTBT) (Fig. 1). Its thermal stability and phase behaviour were investigated by DSC, TGA, SAXS and WAXS methods. The solubility of EH-P-BTBT is an order of magnitude higher than those for its analogue with linear n-hexyl groups C8-P-BTBT with the average field-effect mobility $\mu = 0.6 \text{ cm}^2/\text{Vs}$.¹ The devices were manufactured using two different solution processing methods: doctor blade (DB) and spin-coating (SC). DB layers were obtained at two different speed modes, previously demonstrated their effectiveness – 0.3 and 10 mm/s.^{2,3} To optimize the application conditions, the solutions were made in various solvents with different boiling points – toluene (111 °C), o-xylene (144 °C) and 1,2-dichlorobenzene (DCB; 179 °C). The films obtained from DCB were uneven over the entire surface due to dewetting. The maximum effective $\mu = 2.4 \times 10^{-3} \text{ cm}^2/\text{Vs}$ was achieved from SC devices prepared from toluene solution. Their thermal annealing near the crystal to SmA mesophase transition temperature (225 °C) led to a decrease in the film roughness (from 1.6 to 0.9 nm), but the devices did not work. Solvent vapor annealing in heptane led to a film separation and a decrease in mobility by an order of magnitude. Thus, introduction of branched 2-ethylhexyl substituents to P-BTBT core leads to significant increase in solubility, but decrease in mobility due to change in the crystal packing.

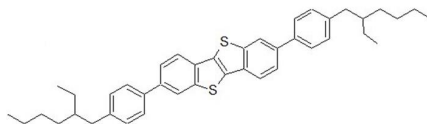


Figure 1. The chemical structure EH-P-BTBT.

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).

¹ Borshchev O.V. et al. *J. Mater. Chem. C*. 2025, **13**, 17728-17737.

² Levkov L. L. et al. *Materials*. 2025, **18**, 743.

³ Shaposhnik P. A. et al. *Dokl. Phys. Chem.* 2021, **496**, 20-24.

Donor–Acceptor Conjugated Polymers Absorbing in the Second Near-Infrared Transparency Window for Biomedical Applications

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The search for non-invasive methods for the deep diagnosis and therapy of malignant tumors remains one of the priority tasks of modern medicinal chemistry. Conventional approaches are associated with a high risk of side effects and insufficient selectivity. Optical methods, such as phototherapy and tumor bioimaging, are regarded as a promising alternative, but their efficiency is largely determined by the penetration depth of radiation into tissue. At present, most photoactive agents operate within the first near-infrared window (NIR-I, 650–950 nm), where the penetration depth is limited by tissue light scattering and by light absorption from blood components, hemoglobin, melanin, and water.

Shifting the absorption of an organic chromophore into the second near-infrared window (NIR-II, 1000–1700 nm) without loss of biocompatibility can be achieved through donor–acceptor (D–A) design of conjugated polymers. The combination of donor and acceptor units induces charge transfer, narrows the energy gap, and shifts absorption toward longer wavelengths¹.

In this work, this strategy is implemented for a series of conjugated D–A polymers based on a common thiadiazoloquinoxaline acceptor core combined with different donor units. The physicochemical properties of the polymers and of the nanoparticles prepared from them were investigated, and all of the polymers were shown to absorb within the second near-infrared window. The average hydrodynamic diameters of the resulting nanoparticles reached up to 150 nm. The cytotoxicity of the series toward tumor cells was also evaluated in vitro, which together allows the potential of the series as phototherapy and bioimaging agents to be assessed.

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¹ Ji Y. et al. *Coordination Chemistry Reviews*. 2026, **552**, 217507.

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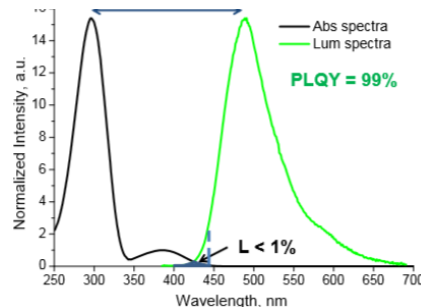
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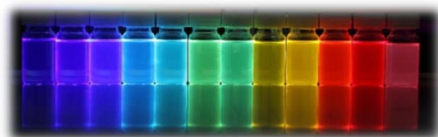
The main goal of LumInnoTech is research, development and commercialization of Nanostructured Organosilicon Luminophores (NOLs) with unique optical properties combining those of organic luminophores and inorganic quantum dots.

Key advantages of NOLs:

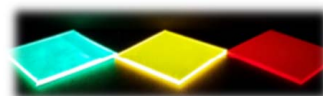
- High luminescence quantum yield: up to 99%
- High molar extinction coefficient: up to 300 000
- Large pseudo Stokes shift: up to 250 – 300 nm
- The possibility of controlling a wavelength of the light emission in a wide range
- Good solution processability
- High stability



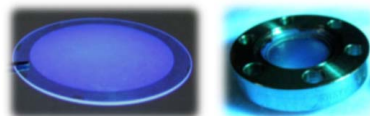
➤ **A library of NOLs, emitting at the desired wavelengths in the range from 390 to 650 nm.**



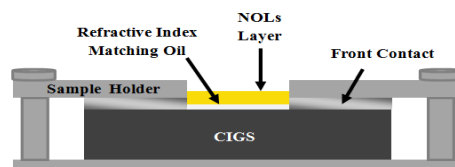
➤ **Wavelength shifting plates for pure CsI crystals**



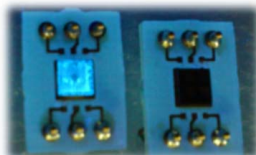
➤ **VUV wavelength shifters for improving photon detection efficiency of noble gas detectors**



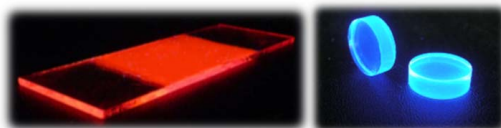
➤ **Luminescent Down Shifting Materials for CIGS Photovoltaics**



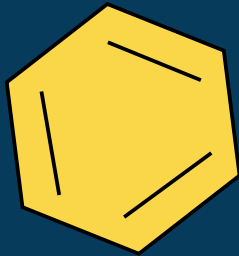
➤ **Effective Spectral Shifters for Silicon Photomultipliers**



➤ **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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