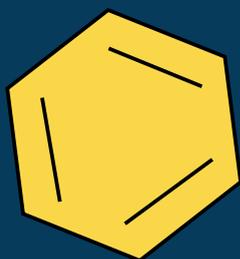




10<sup>th</sup> International Fall School  
on Organic Electronics

Book of Abstracts



September 22-26, 2024  
Moscow region, Russia  
Hotel Soyuz  
<http://www.ifsoe.ru>

# 10<sup>th</sup> INTERNATIONAL FALL SCHOOL ON ORGANIC ELECTRONICS – 2024 (IFSOE-2024)

## 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)

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## 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 10<sup>th</sup> International Fall School on Organic Electronics – 2024 Time Schedule

Moscow, Russia (GMT+3)

	Sunday September 22nd	Monday September 23rd	Tuesday September 24th	Wednesday September 25th	Thursday September 26th			
	<i>School</i>							
9:00		Sergey Ponomarenko	Dmitry Paraschuk	Maxim Kazantsev	Vladimir Dyakonov	9:00		
10:00		Pavel Troshin	Johannes Gierschner	Marta Mas-Torrent	Alessandro Troisi	10:00		
		Jie Min	Surya Prakash Singh	Oleg Borshchev	Jian Liu			
11:00		Leonid Kulik	Alexander Yakubovich	<u>Oral talks 4</u>	<u>Oral talks 6</u>	11:00		
	Coffee-break							
12:00	Registration at ISPM RAS 16:00 Departure to Conference site	Han Yan	Alexey Tameev	Roland Resel	School Closing	12:00		
		<u>Oral talks 1</u>	<u>Oral talks 3</u>	Mikhail Khrizanforov				
13:00		Lunch				13:00		
14:00		Lunch				14:00		
15:00		Yuriy Luponosov	Trip to New Jerusalem (optional) / Sport activities	Zhengxu Cai	14:30 Departure to Moscow	15:00		
		Carlos Graeff		<u>Oral talks 5</u>				
16:00		<u>Oral talks 2</u>					16:00	
	Coffee-break							
17:00	Hotel arrival.	<u>Poster session 1</u>	Evening lecture	<u>Poster session 2</u>			17:00	
18:00	Registration							
19:00	Dinner			Conference dinner	19:00			
20:00	Opening ceremony <u>Vitaly Podzorov</u>	Moscow sightseeing tour	Sport activities		20:00			
21:00	Welcome-party		Leisure time		21:00			
22:00-22:30							22:00-22:30	

## Sunday, September 22<sup>nd</sup>

12:30 – 16:00	<b>Registration at ISPM RAS. Departure to conference site</b>
17:00 – 19:00	<b>Hotel arrival. Registration.</b>
19:00 – 20:00	<b>Dinner</b>
20:00 – 20:15	<b>School opennig</b>
20:15 – 21:00	<b>T-1. Vitaly Podzorov.</b> High-Resolution ac-Hall Effect Measurements of Charge Transport Properties of Emergent Materials
21:00 – 22:30	<b>Welcome-party.</b>

## Monday, September 23<sup>rd</sup>

8:00 – 9:00	<b>Breakfast</b>
	Chair: <i>Yuriy Luponosov</i>
9:00 – 9:45	<b>T-2. Sergey Ponomarenko.</b> Annulated Small Molecules, Oligomers and Polymers in Organic Electronics
9:45 – 10:30	<b>T-3. Pavel Troshin.</b> Probing Intrinsic Photochemical Stability and Radiation Hardness of Organic Semiconductors: New Lessons we Learned From Materials Chemistry
10:30 – 11:00	<b>I-1. Jie Min.</b> Modification of Metastable Phase in Organic Solar Cells
11:00 – 11:30	<b>I-2. Leonid Kulik.</b> Volatile and Non-Volatile Additives to Active Layer of Organic Solar Cells
11:30 – 12:00	<b>Coffee-break</b>
	Chair: <i>Pavel Troshin</i>
12:00 – 12:45	<b>T-4. Han Yan.</b> Spontaneous Charge Photogeneration in Non-Fullerene Acceptor: Discovery and Potential Application
	<b>Oral talks 1.</b>
12:45 – 13:00	<b>O-1. Alina Sonina.</b> Template-Induced Crystallization of Novel Orthorhombic 9,10-Diphenylanthracene Polymorph
13:00 – 13:15	<b>O-2. Valeriy Postnikov.</b> On the Influence of the Molecular Structure of Linear Thiophene-Phenylene Oligomers with a Central Benzothiadiazole Fragment on the Growth, Structure and Properties of Crystals
13:15 – 13:30	<b>O-3. Georgiy Yurasik.</b> Crystals of 4,7-di-2-thienyl-2,1,3-benzothiadiazole and its Derivatives with Terminal Trimethylsilyl and Alkyl Substituents: Synthesis, Growth, Structure, Electrical and Optical-Fluorescent Properties
13:30 – 14:30	<b>Lunch</b>

	Chair: <i>Jie Min</i>
14:30 – 15:00	<b>I-3.</b> <i>Yuriy Luponosov.</i> Development of Conjugated Donor-Acceptor Molecules for Organic and Perovskite Optoelectronics
15:00 – 15:30	<b>I-4.</b> <i>Carlos Frederico de Oliveira Graeff.</i> $\text{Ti}_3\text{C}_2\text{T}_x$ MXene for Efficient and Stable Perovskite Solar Cells
	<b><u>Oral talks 2.</u></b>
15:30 – 15:45	<b>O-4.</b> <i>Azat Akbulatov.</i> The Impact of ZnO Surface on the Stability of Perovskite Films and Solar Cell
15:45 – 16:00	<b>O-5.</b> <i>Danila Saranin.</i> Towards Adaptation of the Industrial Requirements for Up-Scaling of Perovskite Solar Modules
16:00 – 16:15	<b>O-6.</b> <i>Dmitriy Shikin.</i> New Non-Fused Asymmetric Nonfullerene Acceptors for Polymer Solar Cells
16:15 – 16:30	<b>O-7.</b> <i>Polina Sukhorukova.</i> Self-Assembled Monolayer Materials Based on Triphenylamine with Anchor Groups for Perovskite Solar Cells
16:30 – 17:00	<b>Coffee-break</b>
17:00 – 19:00	<b><u>Poster session 1 (P-1 – P-18)</u></b>
19:00 – 20:00	<b>Dinner</b>
20:00 – 23:00	<b>Moscow sightseeing tour (optional)</b>

## Tuesday, September 24<sup>th</sup>

8:00 – 9:00	<b>Breakfast</b>
	Chair: <i>Sergey Ponomarenko</i>
9:00 – 9:45	<b>I-5.</b> <i>Dmitry Paraschuk.</i> Non-Radiative Processes in Organic Luminophores
9:45 – 10:30	<b>T-6.</b> <i>Johannes Gierschner.</i> Color-Pure All-Organic Emitter Design on Physical Grounds
10:30 – 11:00	<b>I-5.</b> <i>Surya Prakash Singh.</i> $\pi$ -Conjugated Small Molecules: Rational Design, Synthesis and their Applications in Photonic Devices
11:00 – 11:30	<b>I-6.</b> <i>Alexander Yakubovich.</i> Computational Discovery of Materials for Deep Blue PHOLED Emitters
11:30 – 12:00	<b>Coffee-break</b>
	Chair: <i>Dmitry Paraschuk</i>
12:00 – 12:30	<b>I-7.</b> <i>Alexey Tameev.</i> Photo- and Electrical Features of Semisynthetic Macrocyclic Compounds

	<b><u>Oral talks 3.</u></b>
12:30 – 12:45	<b>O-8.</b> <i>Nikita Dubinets.</i> Multiscale Quantum Chemical Calculations of Highly Efficient Narrowband Deep-Blue Fluorophores
12:45 – 13:00	<b>O-9.</b> <i>Vladimir Nikitenko.</i> Geminate Recombination Kinetics in Organic Semiconductors, Controlled by Extremely Non-Equilibrium Hopping Transport
13:00 – 13:15	<b>O-10.</b> <i>Anna Saunina.</i> Analytical Modeling of Hopping Transport of Charge Carriers and Excitations in Materials with Correlated Disorder
13:30 – 14:30	<b>Lunch</b>
14:30 – 17:30	<b>Trip to New Jerusalem (optional)</b>
14:30 – 17:30	<b>Sport activities</b>
16:30 – 17:30	<b>Coffee-break</b>
17:45 – 19:00	<b>Evening lecture.</b> <i>Mikhail Nechaev.</i> A Guide to Quickly Writing a PhD Thesis
19:00 – 20:00	<b>Dinner</b>
20:00 – 21:00	<b>Sport activities / Leisure time</b>

## Wednesday, September 25<sup>th</sup>

8:00 – 9:00	<b>Breakfast</b>
	Chair: <i>Zhengxu Cai</i>
9:00 – 9:45	<b>T-7.</b> <i>Maxim Kazantsev.</i> Controlling the Structure and Functional Properties of Crystalline Organic Materials
9:45 – 10:30	<b>T-8.</b> <i>Marta Mas-Torrent.</i> Organic Field-Effect Transistors: Crystal Structure/ Performance Correlations
10:30 – 11:00	<b>I-8.</b> <i>Oleg Borshchev.</i> Synthesis and Properties of Thiophene/Phenylene Co-Oligomers for Organic Electronics and Photonics
	<b><u>Oral talks 4.</u></b>
11:00 – 11:15	<b>O-11.</b> <i>Andrey Sosorev.</i> Impact of Electronegative Atoms on Dynamic Disorder in Crystalline BTBT Derivatives
11:15 – 11:30	<b>O-12.</b> <i>Askold Trul.</i> Electronic Nose Based on Siloxane Derivatives of BTBT with Different Length of Terminal Alkyl Group
11:30 – 12:00	<b>Coffee-break</b>
	Chair: <i>Askold Trul</i>
12:00 – 12:45	<b>T-9.</b> <i>Roland Resel.</i> Film Structure by X-ray Diffraction Methods: The Example of OEG-BTBT
12:45 – 13:15	<b>I-9.</b> <i>Mikhail Khrizanforov.</i> Expanding the Scope of Electrochemistry: Methods and Applications

13:15 – 13:30	<b>I-10.</b> <i>Alexei Komolov.</i> Electron Spectroscopy Investigation of Energy Band Profiles of Conjugated Molecular Films on Semiconductor and on Metal Oxide Surface
13:30 – 14:30	<b>Lunch</b>
	Chair: <i>Carlos Frederico de Oliveira Graeff</i>
14:30 – 15:15	<b>T-10.</b> <i>Zhengxu Cai.</i> Host-Guest Doping Systems Towards Organic Room-Temperature Phosphorescence
	<b>Oral talks 5.</b>
15:15 – 15:30	<b>O-13.</b> <i>Gagik Ghazaryan.</i> A Close Look at Dielectric Elastomer Actuators
15:30 – 15:45	<b>O-14.</b> <i>Oleg Kharlanov.</i> Intermolecular Interaction Energy-Based Computational Screening of High-Mobility Organic Semiconductors
15:45 – 16:00	<b>O-15.</b> <i>Polina Shaposhnik.</i> Towards the High Shelf Life Stability of BTBT Semiconductor Materials
16:00 – 16:15	<b>O-16.</b> <i>Vadim Krylov.</i> The Design of Bio-Recognizing Surfaces for Application in Sensors for Fungal Pathogen Detection
16:15 – 16:30	<b>O-17.</b> <i>Elena Poimanova.</i> Universal Approach to Fabrication of Reusable EGOFET Aptasensors Based on Track Membranes
16:30 – 17:00	<b>Coffee-break</b>
17:00 – 19:00	<b>Poster session 2 (P-19 – P-36)</b>
19:00 – 23:00	<b>Conference Dinner</b>

## Thursday, September 26<sup>th</sup>

8:00 – 9:00	<b>Breakfast</b>
	Chair: <i>Maxim Kazantsev.</i>
9:00 – 9:45	<b>T-11.</b> <i>Vladimir Dyakonov.</i> Efficiency-Limiting Pathways in Organic Materials and Opto-Electronic Devices - the Role of Triplets
9:45 – 10:30	<b>T-12.</b> <i>Alessandro Troisi.</i> Digital Materials Discovery in Organic Electronics
10:30 – 11:00	<b>I-11.</b> <i>Jian Liu.</i> n-Type Organic Ionic-Electronic Mixed Conductors for Electronic Devices
	<b>Oral talks 5.</b>
11:00 – 11:15	<b>O-18.</b> <i>Abhay Sagade.</i> Engineering Performance of High-Frequency Organic Electronic Devices
11:15 – 11:30	<b>O-19.</b> <i>Tao Wang.</i> The Design and Application of Organic Room-temperature Phosphorescent Materials
11:30 – 12:00	<b>Coffee-break</b>

12:00 – 13:00	<b>School closing</b>
13:00 – 14:30	<b>Lunch / Hotel check out</b>
14:30 – 14:45	<b>Departure to Moscow</b>

## Poster session 1

Monday, September 23<sup>rd</sup>, 17:00

Bobrova, Elizaveta A.	P1	Synthesis and Properties of New BTBT Derivatives for Organic Electronics
Cheshkina, Darya S.	P2	Synthesis and Aggregation-Induced Emission of 1,4-bis((9H-diazafluoren-9-ylidene)methyl)phenylenes
Chuyko, Irina A.	P3	Synthesis of Conjugated Polymers Based on Triphenylamine for Application in Perovskite Solar Cells and Metal-Ion Batteries
Dominskiy, Dmitry I.	P4	Tuning Molecular Packing and Charge Transport in Thiophene-Phenylene Co-Oligomer Single Crystals for Field-Effect Devices
Fedorenko, Roman S.	P5	Thiophene-Phenylene Co-Oligomers for Organic Field-Effect Phototransistors
Filipenkov, Dmitry A.	P6	Influence of Charge Carrier Mobility on the Form of Charge Carrier Recombination Rate Spatial Distribution in Organic Light Emitting Diodes
Gradova, Anna V.	P7	Novel Annulated Organic <i>p</i> -Type Semiconductor: Synthesis and Properties
Gudkova, Irina O.	P8	Synthesis Strategy of a Novel Organosilicon Polymer with Dihexyl-Substituted [1]BenzoThieno[3,2-b][1]BenzoThiophene Fragments in the Main Chain
Isaeva, Yulia A.	P9	Nanoparticles Based on Organic Conjugated Donor-Acceptor Molecules for Cancer Phototherapy
Karaman, Polina N.	P10	Biorecognition of Monoclonal Antibodies by EGOFET Based on Oligosaccharides
Khmelnitskaia, Alina G.	P11	Circular Dielectric Elastomer Actuators Based on PDMS/MQ Composites
Kleymyuk, Elena A.	P12	Polyvinylidene Fluoride Grafted with Polyethyl Methacrylate Chains for Pressure Sensors
Koptyaev, Andrey I.	P13	Gentle Substrate Cooling in Vacuum Deposition of Small-Molecules Semiconductors
Krasnikov, Danila A.	P14	The Specificity of the Sensitivity of Organic Field-Effect Transistors with Various Interface Dielectrics
Kravets, Natalia V.	P15	Ternary Composite of Polymer, Fullerene and Fluorinated Multi-Walled Carbon Nanotubes as the Active Layer of Organic Solar Cells
Kretova, Elena A.	P16	I-Motif Aptamer for Biosensing by Electrolyte-Gated Organic Field-Effect Transistors

Kuleshov, Bogdan S.	P17	Crown Ether-Based Electrolyte-Gated Organic Field-Effect Transistor for Detection of Alkali Metals
Titova, Yaroslava O.	P18	Inkjet Printed Organic Semiconductor Devices Based on C8-BTBT Materials

## Poster session 2

Wednesday, September 25<sup>th</sup>, 17:00

Bezsudnov, Igor V.	P19	Conductivity of Filled Polymers Modelled by the Cooperative Systems Approach
Gaikov, Dmitry K.	P20	A new approach to the production of organosilicon photo conversion and photo-curable films
Levkov, Lev L.	P21	Tuning of Physical and Chemical Properties of Dithienyl Derivatives of [1]BenzoThieno[3,2-b] [1]BenzoThiophene by Variation of the Position of Solubilizing Alkyl Groups
Mannanov, Artur L.	P22	Blue Organic Light-Emitting Diodes Based on New Multi-Resonance Fluorescence Materials
Mikhailov, Maxim S.	P23	Indolocarbazole- and Diindolophenazine-Based Fluorophore with High-Efficiency Blue Electroluminescence
Molchanov, Ivan A.	P24	Tuning the Morphology of PM6/Y6 Active Layer of Organic Solar Cells via Intermediate Ternary Donor/Acceptor/Volatile Additive Blend
Moshkina, Tatiana N.	P25	Catalyst-Free Synthesis of Carbazolyl-Containing Fluorophores as Perspective Functional Materials
Papkovskaya, Elizaveta D.	P26	Synthesis and Properties of New Non-Fullerene Acceptors for Organic Solar Cells
Poletavkina, Liya A.	P27	Synthesis and Structure-Property Relationship Study for New Push-Pull Fused Oligomers Based on Indole[3,2-b]Indole and BenzoThieno[3,2-b]BenzoThiophene
Polyakov, Roman A.	P28	Novel Luminescent Polymers for 3 <sup>th</sup> Generation OLED Materials
Popova, Vlada V.	P29	Study of Influence of Terminal Groups in 2,1,3 Benzothiadiazole-Based Thiophene Phenylene Derivatives
Sorokina, Ekaterina A.	P30	Synthesis of Organosilicon Copolymers with Grafted Biotin-Containing BTBT Segments
Stakanova, Daria E.	P31	Novel Luminophores Based on 2,1,3-Benzothiadiazole Containing Phenyl, Thiophene and Various Terminal Substituents
Tolkachev, Egor D.	P32	Synthesis and Optoelectronic Properties of Thiophene-Containing Derivatives of Tris(2,4,6-Trichlorophenyl)Methyl Radical
Trofimova, Kristina E.	P33	Experimental and Calculated Electronic Structure of Organic Semiconductors Based on Benzothienoacene
Trukhanov, Vasiliy A.	P34	Modeling the Charge Traps Influence on Organic Phototransistor Performance with Spatially Localized Photoelectric Effect
Zaborin, Evgeniy A.	P35	Synthesis and Properties of Novel Polysiloxanes Grafted with Dialkyl BTBT Derivatives
Balakirev, Dmitry O.	P36	Triphenylamine-based Push-pull Small Molecules as a Platform for Elaborating Organic Semiconductor Materials with Wide Applications Range

# Tutorial lectures

## ***ac*-Hall Measurements of Charge Carrier Transport in Organic and Hybrid Semiconductors**

*V. Podzorov*<sup>1\*</sup>

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The importance of Hall effect in evaluating the charge transport of novel materials is recognized in materials science, semiconductor physics, and electronics. Advantages of Hall measurements include: (a) direct access to the mobile carrier concentration and mobility in a steady-state transport regime; (b) providing an alternative for mobility evaluation in systems where other techniques fail; (c) offering means of distinguishing between different transport mechanisms (e.g., hopping, band-like, or their combination); and (d) ability to disentangle contributions of various carrier types or trap states. However, in low-mobility materials, the conventional (that is, *dc*) Hall measurements are extremely challenging. High-resolution *ac*-Hall and photo-Hall methods, recently developed in our group, have resulted in a significant progress in this direction in organic semiconductors and lead-halide perovskites.<sup>1,2</sup> In this lecture, I will discuss a few examples of the transport physics studies using the Hall measurements. For instance, such measurements helped to elucidate the role of grain boundaries in high-performance polycrystalline organic transistors, where capacitively charged grain boundaries lead to an “underdeveloped” Hall effect.<sup>3</sup> In another example, the *intrinsic* mobility-strain relationship has been experimentally revealed in organic semiconductors for the first time, achieved via simultaneous field-effect transistor (FET) and gated-Hall measurements under a uniaxial strain in ultra-thin and flexible, single-crystal rubrene FETs.<sup>4</sup> These measurements reveal an anisotropic and reversible modulation of charge mobility with strain. A photo-Hall effect has also been recently measured in organic semiconductors, where it was possible to correctly disentangle the mobilities and densities of the photogenerated charges.<sup>2</sup> Among other insights, the photo-Hall effect measurements performed in high-mobility rubrene single crystals confirmed our previous findings that photoconductivity in this material is due to the interaction of long-lived mobile triplet excitons with the crystal’s surface.<sup>5,6</sup> Finally, high-resolution *ac*-Hall measurements have proven to be very useful in the investigation of the intrinsic (trap-free) charge transport of epitaxial crystalline perovskite transistors.<sup>7</sup>

*This work was partially supported by the Donald H. Jacobs Chair in Applied Physics at Rutgers University, the U.S. National Science Foundation under the grant ECCS-1806363, and the Rutgers initiative for Materials Research (iMR) seed grant 300761.*

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<sup>1</sup> Chen, Y., Yi, H. T., Podzorov, V., *Phys. Rev. Applied* 2016, **5**, 034008.

<sup>2</sup> Bruevich, V., Choi, H. H., Podzorov, V., *Adv. Funct. Mater.* 2021, **31**, 2006178.

<sup>3</sup> Choi, H. H., Paterson, A. F., Fusella, M. A., Panidi, J., Solomeshch, O., Tessler, N., Heeney, M., Cho, K., Anthopoulos, T. D., Rand, B. P., Podzorov, V., *Adv. Funct. Mater.* 2020, **30**, 1903617.

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## Annulated Small Molecules, Oligomers and Polymers in Organic Electronics

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Organic electronics growing very fast due to design and developing of novel functional materials as well as device structures optimization. Such advantages of organic electronics as light weight and flexibility originates from intrinsic properties of organic semiconductors, which are  $\pi$ -conjugated organic molecules, oligomers or polymers. Conjugation means the presence of  $\pi$ -orbitals delocalized over the whole or a part of a molecule containing linearly conjugated or annulated (hetero)aromatic rings.

Nowadays, annulated small molecules, oligomers and polymers containing annulated fragments are increasingly used as semiconductor materials in organic electronics. This is due to the fact that annulation, unlike linear conjugation, forms more rigid molecular fragments with both stronger intermolecular interaction and fewer vibrational and rotational degrees of freedom, which reduces dynamic disorder and leads to an increase in the main characteristic of semiconductors – charge carrier mobility.

In the lecture a classification of different annulated fragments and molecules will be introduced, examples of their synthesis<sup>1,2</sup> will be given and application in various organic electronics devices – organic field-effect transistors (OFETs) and gas sensors based on them<sup>3</sup>, organic light-emitting transistors (OLETs)<sup>4</sup>, electrolyte-gated organic field-effect transistors (EGOFETs)<sup>5</sup> and biosensors based on them<sup>6,7</sup>, organic photovoltaics<sup>8,9</sup> and perovskite solar cells<sup>10</sup> – will be presented. A particular attention will be devoted to comparison of the properties of different annulated molecules with their linearly conjugated analogs.

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## Probing Intrinsic Photochemical Stability and Radiation Hardness of Organic Semiconductors: New Lessons we Learned From Materials Chemistry

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In this report, we will focus on major challenges in the investigation of intrinsic stability of organic semiconductor materials used as absorber components in organic solar cells. Starting from the discussion of general research methodology we will proceed to feature the main discoveries in this field such as dominant aging pathways and molecular structure effects on the material photochemical behavior. In the second part, we will present the results of our systematic study of a broad panel (>300 structures) of conjugated polymers and small molecules, including fullerene derivatives and non-fullerene acceptors (NFAs) in the context of their stability with respect to UV light and gamma-rays. Important correlations between the materials' stability, their chemical compositions and molecular structures will be presented. A prognostic model enabling the prediction of photostability of arbitrary chosen conjugated polymer structures will be introduced and the limitations of the model will be considered. The guidelines for rational design of new absorber materials for stable and efficient organic photovoltaics will be formulated based on explicit experimental evidence. Finally, the degradation behavior of organic solar cells under exposure to UV-light and gamma-rays will be analyzed and the conclusions on the suitability of this technology for space applications will be drawn.

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## Spontaneous Charge Photogeneration in Non-Fullerene Acceptor: Discovery and Potential Application

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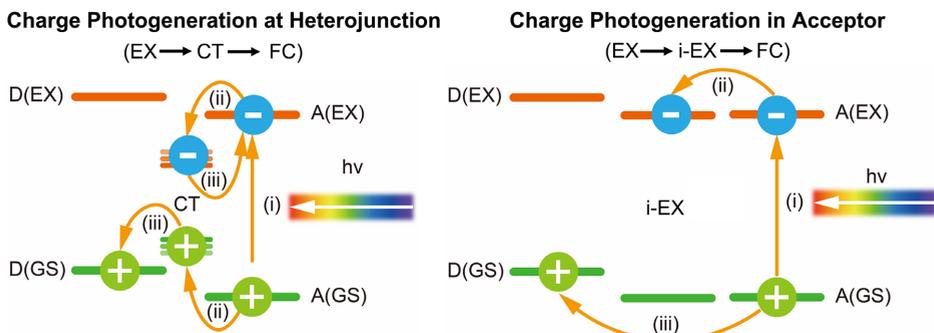


Fig. 1. Scheme of two kinds of charge photogeneration routes

Efficient charge photogeneration is the core issue in the operation of organic solar cell (OSC). It is widely accepted that the single exciton (EX) will split into charge transfer (CT) exciton at the donor/acceptor (D/A) heterojunction before free charge (FC) formation. Nowadays, the traditional view is challenged by new observations in state-of-the-art non-fullerene acceptors (NFAs).<sup>1</sup> Theoretical calculation predicts that the EX binding energy of NFAs is significantly reduced to room-temperature thermal energy by polarized energy. Then scientists observed an intra-moiety exciton (i-EX) signal by the transient absorption spectroscopy in infrared range. The i-EX can spontaneously transform into FC in neat NFA films. Therefore, the charge photogeneration seems getting rid of the heterojunction CT exciton in NFAs. The spontaneous charge photogeneration inspires the developments of semitransparent and single-component OSCs. The recent progresses in these two fields will be introduced.

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## Non-Radiative Processes in Organic Luminophores

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Efficient organic luminophores emitting light in the visible and infrared spectral ranges are in great demand for organic optoelectronic devices, e.g. for light-emitting diodes. Usually, a number of non-radiative (NR) processes, e.g. internal conversion and intersystem crossing, accompany light emission affecting its quantum yield, spectrum, and transient behaviour. On the other hand, NR-processes in molecules are totally controlled by their motion, specifically by vibrations. As a result, to find efficient luminophores, one needs to identify robust structure-property relations that can direct smart design of efficient organic luminophores for various applications.

In this tutorial, we review and critically analyse the basic concepts that underpin our knowledge about the NR-processes and their interplay with light emission in organic luminophores. We analyse how radiative and non-radiative processes compete so that the fastest one dominates in relaxation of the electronic excitation. We start with fundamental relationship determining the radiation rate of a quantum system and then add molecular vibrations according to adiabatic approximations, specifically the Born-Oppenheimer one. Then we consider the concepts of ultrafast vibrational energy relaxation and come to Vavilov-Kasha and Vavilov's rules.

The models for internal conversion are reviewed, which is essentially a non-adiabatic process allowing transition between the different electronic states. The notion of accepting and promoting modes and the corresponding symmetry restrictions are discussed. The so-called energy-gap law is presented and critically analysed. Furthermore, we present the modern understanding of intersystem crossing and reverse intersystem crossing, which apart from internal conversion are mediated by spin-orbit coupling.

We review experimental techniques that can provide information about the NR-processes, specifically photoluminescence and transient absorption spectroscopies. The effects of luminophore molecular environment and their contribution to the NR-processes are discussed.

Finally, we discuss how quantum chemistry techniques can help us to model the NR-processes at the atomistic level and map them to the specific structure of organic luminophores. We conclude that deeper understanding of NR-processes is necessary to promote the development of stable organic luminophores for various applications.

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

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## Color-Pure All-Organic Emitter Design on Physical Grounds

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Color-pure blue  $\pi$ -conjugated all-organic emitters have raised considerable interest for ultra-high definition organic LED displays in recent years. However, rational molecular design concepts beyond phenomenological approaches are largely missing. Here, we reveal how color-pure blue all-organic emitters can be understood and constructed on physical grounds. For this, we first classify spectral width, demonstrating the need for a more differentiated picture than commonly perceived. We then categorize, in a rigorous manner, all factors which contribute to spectral broadening processes of conjugated organic compounds. With this at hand, we establish general structure-property relationships for blue emitters with narrow band widths, deducing specific design rules, which were not inherently understood by now. We show that this rational concept is fundamentally different from those, which can be deduced for pure-color emitters in the green to red spectral region. The simple and clear design rules derived from this concept allow to extend the known chemical space by new structural motifs. Based on this design checklist, we have systematically synthesized a set of blue emitters with  $\lambda_{\text{max}}$  ranging from 440 to 455 nm, exhibiting a spectral width of down to  $760 \text{ cm}^{-1}$  (15 nm). TD-DFT calculations allow for a full rationalization of the observed spectral properties. Their color-pure blue fluorescence, together with good processability, emission lifetimes of 5-8 ns and quantum yields of up to unity makes the novel compounds highly attractive candidates for OLED applications.

## Controlling the Structure and Functional Properties of Crystalline Organic Materials

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Organic highly-emissive materials are demanded in optoelectronics for application in light-emitting diodes, transistors, lasers and sensors.<sup>1</sup> Crystalline materials based on linear conjugated small-molecules containing phenylene, thiophene, furan and fluorene moieties are the most prospective for these applications. Particularly, oligoarylene-phenylenes<sup>2</sup> demonstrated a lucky combination of high solid-state luminescence and charge transport. Introduction of heterocycles or terminal substituents,<sup>3</sup> directed crystallization,<sup>4</sup> polymorphism and molecular doping<sup>5</sup> were demonstrated to be the most powerful approaches for crystal structure, luminescence and semiconductor characteristics control. 9H-fluoren-9-ylidene derivatives,<sup>6</sup> including ((9H-(diazfluorene)-9-ylidene)methyl)arylenes,<sup>7</sup> exhibit aggregation-induced emission coupled with sensory properties due to solid-state conformational rearrangements. The introduction of nitrogen atoms into the fluorene core also enhances electron-withdrawing effect and brings a chelating ability resulting in the formation of coordination polymers having porous structure, luminescence and being sensitive to dehydration.

Here, we discuss the synthetic, crystal-engineering and physico-chemical approaches for molecular and crystal structure control allowing tuning the luminescence, charge transport and sensory response.

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

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## Organic Field-Effect Transistors: Crystal Structure/Performance Correlations

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Organic printed electronics is an emerging field for device technology. Despite the impressive charge carrier mobilities that have been reported for organic field-effect transistors (OFETs) in recent years, it is still a challenge to achieve highly reliable devices fabricated using low-cost solution-based techniques. For this purpose, it is necessary to fabricate thin-films controlling the thin film morphology and structure as well as to optimise the device interfaces. We will here overview the working principle of OFETs and the main aspects that have to be considered to optimise the device performance.

Further, recently, we have shown that the use of blends of small molecule organic semiconductors (OSCs) with polystyrene deposited with a solution shearing technique, is a promising route to realise OFETs at low cost and with high mobility and stability.<sup>1-2</sup> We will also show that this approach is a practical and effective means to control OSC polymorphism and achieve long-term device stability with promising metastable polymorphs (Fig. 1). By modifying the ink formulation of the deposition parameters the thin film features can be modified and the device performance improved. In addition, the control of the thin film micro-structure has also an impact in applications, such as for the development of OFETs as X-ray detectors with high sensitivity.<sup>3</sup>

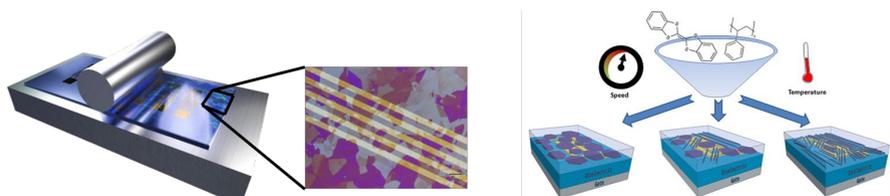


Fig. 1. Deposition of a OSC thin film using a solution-shearing technique (left) and illustration of the control of the thin film morphology/structure by the modification of the ink formulation or deposition parameters (right).

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## Thin Film Structure by X-ray Diffraction Methods: The Example of OEG-BTBT

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The class of benzothieno-benzothiophene (BTBT) molecules has gained a lot of interest, since excellent performance is observed in thin film transistors. Here we report on a specific derivative of BTBT type molecules with oligo-ethylene side chains. Thin films are prepared by spin coating from chloroform solutions and by physical vapour deposition. Detailed characterisation of the thin film morphology is performed by X-ray reflectivity (Figure 1). It is found that the first monolayers at substrate surfaces show different molecular arrangements.<sup>1</sup>

Multiple attempts to get functioning transistor devices based on solution processed films failed. But thin film transistors based on physical vapour deposited thin films show weak device performance with charge mobilities in the range of  $10^{-3}$  cm<sup>2</sup>/Vs.<sup>2</sup>

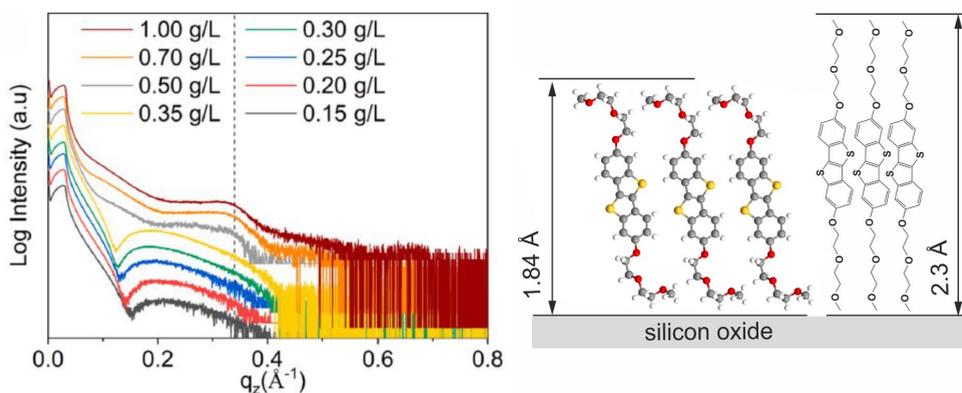


Fig. 1 Left: X-ray reflectivity study of spin coated thin films as a function of different dissolution concentrations. Right: Two different types of molecular packing of the molecule OEG-BTBT within the first monolayer.

We investigated also the phase behaviour of this molecule by polymorph screening, three phases are found.<sup>3</sup> Including surfaces into the polymorph screening process, revealed additional four phases.<sup>4</sup> An unknown mechanism for a melt memory effect was detected which is associated to a strong interaction of the solvent with the oligoethylene side chains of the molecule.<sup>5</sup>

Based on this outstanding structural properties of the molecule OEG-BTBT a tutorial lecture will be presented which gives an introduction to X-ray based methods for the characterization of thin films used in organic electronic devices.

*The work was funded by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 811284 (UHMob).*

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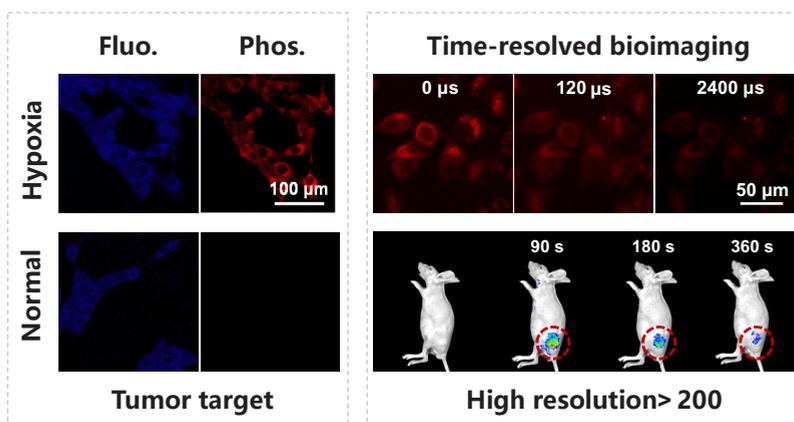
## Host-Guest Doping Systems Towards Organic Room-Temperature Phosphorescence

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Organic room temperature phosphorescent (RTP) materials have wide applications in the fields of smart anti-counterfeiting, information storage, and biological imaging due to their long luminescence lifetime, large Stokes shift, and low biotoxicity. However, it is great challenging to develop organic RTP materials due to the inhibition of the intersystem crossing and unstable triplet excitons. Our group focused on the development of high performance (long lifetimes, high quantum yields, and tunable colors) RTP materials based on “host-guest doping method”, achieving a series of innovative results: (1) New strategy for the development of RTP materials with high quantum yield and long lifetime was established. The phosphorescence mechanisms were investigated and multi-stimulus responsive persistent phosphorescence was realized. (2) Fused ring small molecules and polymers with through-space conjugation property were developed to tune the triplet energy levels. This preparation strategy is highly versatile, with a simple process, low raw material costs, good stability (water and oxygen stability), and temperature responsiveness, addressing the current shortcomings of phosphorescent materials. Furthermore, through molecularly controlled assembly, phosphorescent nanoparticles with uniform sizes and long-term stability in water (>10 days) have been prepared. These excellent phosphorescent properties can completely eliminate interference from biological autofluorescence during imaging processes, not only for efficient long-term imaging of tumor cells but also for high contrast imaging of live mice.



### Avoid auto-fluorescence from bio-tissue

Figure 1 Organic RTP materials for high resolution bioimaging.

## Efficiency Losses in Organic Photovoltaic Materials and Solar Cells - the Role of Triplets

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The great progress in organic photovoltaics (OPV) over the past few years has been largely achieved by the development of non-fullerene acceptors (NFAs), with power conversion efficiencies now approaching 20%. To further improve device performance, loss mechanisms must be identified and minimized. Triplet states are known to adversely affect device performance, since they can form energetically trapped excitons on low-lying states that are responsible for non-radiative losses or even device degradation. Using the complementary spin-sensitive methods of photoluminescence, detected magnetic resonance and transient electron paramagnetic resonance supported by transient absorption, exciton paths are deciphered in OPV mixtures using different polymer donors and NFAs. All mixtures show triplet excitons on the NFA arising from nongeminate hole back-transfer as well as intersystem crossing driven by spin-orbit coupling<sup>1</sup>. Identifying these triplet formation pathways in all tested solar cell absorber films highlights the untapped potential for improved charge generation to further increase plateauing OPV efficiencies.

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## Digital Materials Discovery in Organic Electronics

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This talk will provide an overview of the three main approaches used within the group to aid the discovery of new materials (i) traditional bottom up construction of physical models (ii) high-throughput virtual screening (iii) machine learning (ML). The relation between the three approaches will be discussed including a methodology for selecting the best strategy given time and budget constraints. The challenge of dealing with experimental and highly biased datasets and the difficulty of measuring “novelty” of a given ML-based prediction will be discussed. The talk will explore how linking the prediction with the knowledge of the chemical supply chain can substantially shorten the gap between predictions and experimental verification.

# Invited lectures

## Cost-Reduction Pathways of Organic Photovoltaic Active Layers

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Organic photovoltaics (OPVs) have become a potential candidate for clean and renewable photovoltaic productions. Recently developed OPV materials and devices have made great progress in device efficiency (power conversion efficiency (PCE) > 20%) and operational stability ( $T_{80}$  (the time required to reach 80% of the initial PCE) values exceeding 10000 hours). Given these achievements, many researchers have begun to focus on the cost of OPV materials, like the design and synthesis of non-fused small molecule acceptors and polymer donors with simple structures. In this talk, I will systematically examine the current cost drives (see Fig. 1) and potential pathways to reduce the cost of OPV solar modules by constructing a comprehensive bottom-up cost model.<sup>1</sup> Corresponding conceivable pathways for reducing minimum sustainable price (MSP) values are exhibited in Fig. 1. In this roadmap, we separate out the impact of material cost, yield, factory throughput, and module efficiency, but in some cases these may be coupled as expected. Furthermore, we will take some examples to introduce some promising cost-reduction pathways of photoactive layers, mainly including the design and synthesis of polymer donors with simple structures,<sup>2</sup> the high-throughput fabrication of photoactive layers,<sup>3</sup> and the consistency control of large-scale photoactive layer morphology.<sup>4</sup> Overall, this talk underscores the significance of understanding and utilizing the cost-reduction roadmap in facilitating and guiding the development of next-generation OPV materials and devices.

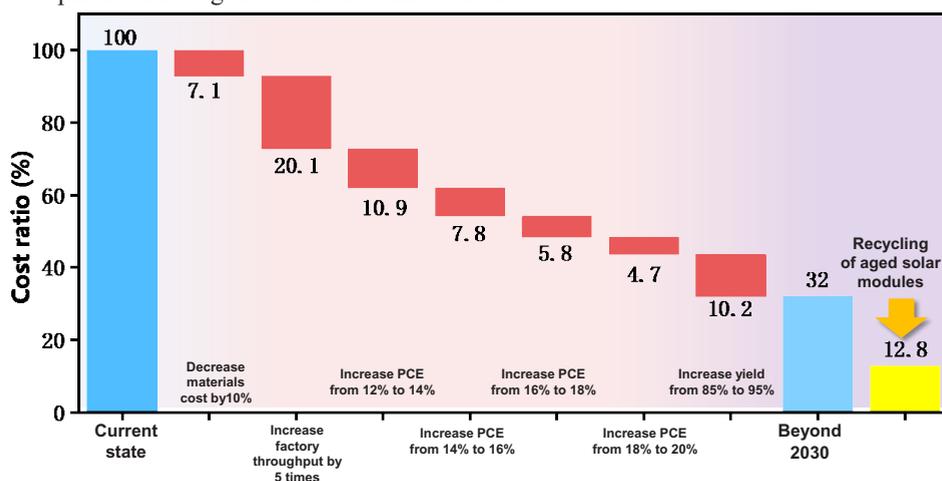


Fig. 1. Roadmap for reducing solar module MSP values of the single-junction solar modules.

*This work was supported by NSFC (project № 22279094 and 223B2904).*

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## Volatile and Non-Volatile Additives to Active Layer of Organic Solar Cells

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Nowadays, organic photovoltaics (OPV) becomes a mature field of renewable energetics, since the power conversion efficiency (PCE) of the laboratory-scale devices approaches 20 %. Despite spectacular PCE growth, the strategy of improving OPV layer component via increasing the complexity of donor and acceptor molecules forming bulk heterojunction active layer has limitations. Therefore, other strategies for improving the performance of OPV devices, in particular, optimization of the morphology of the active layer, are urgently demanded.

Both horizontal and vertical morphology can also be modified with help of various additives, which can be broadly classified into liquid additives, solid volatile additives and non-volatile additives. Liquid additives (also called solvent processing additives), such as diiodooctane or octanedithiol, are added to the solvent and evaporates during spin-coating. For polymer-fullerene composites their main mode of action is selective dissolving of fullerene, which prevents its crystallization and growing of too large fullerene domains <sup>1</sup>. Proper size of both donor and acceptor domains is essential for high yield of exciton splitting and photo-induced charge separation. Volatile solid additives are also dissolved in the solution used for spin coating, but they remain in the donor/acceptor composite after deposition. Most of volatile additives are small organic molecules <sup>2</sup>, although organometallic compounds such as ferrocene sometimes are used. Typically, volatile additives are removed from this composite by subsequent thermal annealing, which is accompanied by change of the molecular packing within donor and/or acceptor domains <sup>3</sup>. This can be used to tune charge transport properties of the composite. Some highly volatile materials, such as naphthalene, do not require thermal annealing, but still enhance stability and reproducibility of organic solar cells. Non-volatile additives, such as carbon nanotubes <sup>4</sup> and graphene-like structures, are also deposited with donor and acceptor. They remain in this ternary donor/acceptor/additive composite and serve as a template for donor and acceptor molecules.

Possibility for improving efficiency, stability and reproducibility, offered by different additives, as well as their disadvantages will be considered.

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## Development of Conjugated Donor-Acceptor Molecules for Organic and Perovskite Optoelectronics

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Organic solar cells (OSCs) and perovskite solar cells (PSCs) have attracted considerable scientific and technological interest compared to conventional photovoltaic technologies based on traditional inorganic semiconductors. Development of new organic semiconductor materials plays a key role in the efficient functioning of both the OSCs and PSCs. For instance, the recent emergence of the new generation of non-fullerene acceptors (NFAs), have revitalized the field of OSCs, with their power conversion efficiency (PCE) rocketing from 11 % to nearly 20 % over the past years. The development of novel suitable dopant-free hole-transport materials is the critical issue for realizing perovskite solar cells with high PCE and long operational lifetimes. The main focus of this lecture will be the demonstration of our recent results in the development of new non-fullerene acceptors<sup>1,2,3,4</sup> for OSCs and hole-transporting materials for PSCs<sup>5,6,7</sup>.

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## Efficient and Stable Perovskite Solar Cells: New Materials and Modeling

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Perovskite solar cells (PSCs) have attracted widespread attention in academia and industry due to their high-power conversion efficiency (PCE) and potential for low-cost, sustainable, and large-scale manufacturing. We have incorporated two-dimensional (2D) materials to enhance the performance of double-cation mixed halide perovskite ( $\text{Cs}_{0.17}\text{FA}_{0.83}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$ ) solar cells. We developed a  $\text{Nb}_2\text{O}_5$  ETL layers adding  $\text{Ti}_3\text{C}_2\text{X}$  MXene into a solution processable ink.<sup>1</sup> The addition of MXene increased the PCE (19.46% for the champion device) and the stability (96% of its original PCE after 500 hours) compared to pristine devices. The improved performance of the  $\text{Nb}_2\text{O}_5$ - $\text{Ti}_3\text{C}_2$  is attributed to the alignment of the energy bands between perovskite and the ETL layer. In inverted or p-i-n PSCs we used an ultra-thin poly(methyl methacrylate) (PMMA) layer to passivate interfacial defects between the perovskite and the ETL layer.<sup>2</sup> With the addition of  $\text{Ti}_3\text{C}_2\text{X}$  MXene resulted in improvement of the PSC photovoltaic parameters, boosting their efficiency to  $21.30 \pm 0.51\%$  (22.1% for the benchmark PSC). The enhanced performance is attributed to a reduction of trap state densities accompanied by mitigation of non-radiative recombination. The PMMA:MX based devices maintained 95% of their original PCE after 3000 h (ISOS-D-11) and took 3X longer to reach T80 compared to the control PSC under heat and light soaking (ISOS-L-2). In another study,<sup>3</sup> the deposition of  $\text{Nb}_2\text{O}_5$  as an electron transport layer via slot die coating was systematically investigated. These Nb 2 5 layers were used as electron transport layers in n-i-p perovskite devices. Current density versus voltage scans were utilized to evaluate the device performance, alongside transient analysis. Under optimal coating conditions, efficiencies up to 12 % were obtained. We will also present a conceptual framework for characterizing photovoltaic devices by integrating cyclic voltammetry (CV) and impedance spectroscopy (IS).<sup>4</sup> This framework is constructed from a microscopic, multi-mode perspective that explicitly accounts for drift, diffusion, displacement, and memory contributions. We derive comprehensive analytical expressions for current-voltage relationships and complex admittance. Our model reveals the inseparable connection between hysteresis behaviors in current-voltage characteristics observed in CV and the apparent capacitive and inductive behaviors seen in IS spectral analysis.

*The authors acknowledge FAPESP (Projects: 2020/12356-8 and 2013/07296-2), FINEP, CAPES and CNPq (INCT NanoVida) for financial support.*

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## $\pi$ -Conjugated Small Molecules: Rational Design, Synthesis and their Applications in Photonic Devices

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Small organic molecules with suitable photophysical and electronic properties have attracted great attention towards Hi-tech applications based on photonic devices, such as dye sensitized solar cells, organic solar cells, emissive displays such as organic light emitting devices; electronic materials, such as organic semiconductors and security printing. Organic solar cells or organic photovoltaics are emerging as one of the promising technologies for renewable energy sources because of their potential low-cost fabrication, color-tunable feature, and mechanical flexibility. Many research activities have endeavoured to develop new organic materials and device configurations for improving the efficiency and practical durability of the devices. Our research groups are actively demonstrating development of new and stable organic molecules for various applications. In this event, I will be presenting our recent development on hole-transport materials for perovskite solar cells. The talk will start with a brief introduction of solar cells followed by industrial application and commercialization of dye molecules. The details of perovskite device using new HTM is depicted in Figure 1.<sup>1</sup>

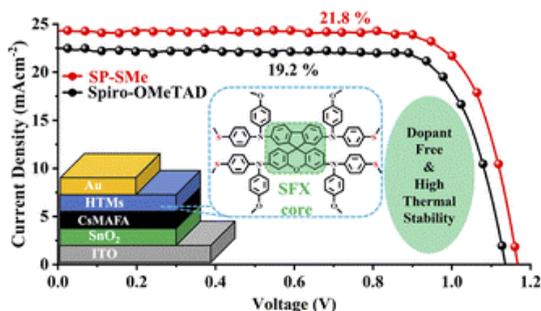


Fig. 1. New HTM for perovskite solar cells

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## Computational Discovery of Materials for Deep Blue PHOLED Emitters

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The rational design of novel materials for organic light-emitting diodes (OLEDs) requires a deep understanding of molecular-scale processes that influence device performance. These include the generation and relaxation of excited states, charge and energy transfer, and photochemical reactions that contribute to material degradation. Computational chemistry provides powerful tools to investigate the properties and morphology of OLED materials, offering insights that are often inaccessible through experimental techniques.

The photoluminescence (PL) efficiency of OLED materials is governed by the balance between radiative and non-radiative relaxation processes within the light-emitting molecule. We discuss a methodology for modeling these competing processes and demonstrate its application in predicting PL quantum yields for a series of Pt(II)-based complexes, offering a framework for designing materials with enhanced emission efficiency.<sup>1</sup>

The discovery and design of deep blue phosphorescent OLED (PHOLED) materials rely heavily on computational methods to study molecular processes such as energy transfer, triplet harvesting, and exciton fusion. Using quantum chemical calculations combined with deep generative models, we explore chemical spaces to identify molecules suitable for triplet-triplet fusion (TTF). A Junction Tree Variational Autoencoder (JT-VAE) and neural networks predict excitation energies, optimizing energy level alignment and significantly accelerating the design process.<sup>2</sup>

Additionally, quantum mechanically derived force fields (QMDF) enable efficient atomistic simulations, allowing the study of material morphology and thermodynamic processes. We apply this methodology to predict the evaporation temperature of organometallic complexes, critical for OLED manufacturing via vapor deposition.<sup>3</sup> Together, these computational tools offer a versatile approach for the rational design of OLED materials, enabling precise control of molecular properties to enhance device performance.

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## Mobility of Charge Carriers in Functional Layers of Perovskite Cells

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The report examines the issue of consistency of charge carrier mobility in perovskite films and adjacent hole and electron transport layers (HTL and ETL, correspondingly). Perovskite diode structures anode/HTL/perovskite/ETL/cathode demonstrate high efficiency of solar cells and photodiodes. The efficiency of perovskite cells is known to exceed 25%<sup>1</sup> and 23%<sup>2</sup> on rigid and flexible substrates, respectively. The mobility of charge carriers in polycrystalline perovskite layers (MAPI and its analogues) ranges widely from 1 to 10<sup>3</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>, while in typical organic materials for HTL and ETL, the mobility has much lower values in the range of 10<sup>-4</sup> ÷ 10<sup>-2</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>. The high values of mobility in perovskite films given in the literature were obtained in most cases using methods that do not register drift mobility.

We performed drift mobility measurements in MAPI films by recording transient currents in a conventional time-of-flight (ToF) experiment and transient space charge-limited currents (DI-SCLC). The obtained values of charge carrier mobility,  $\mu_{\text{per}}$ , are in the range of 10<sup>-2</sup> ÷ 10<sup>-1</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>. It is for these values of drift mobility in perovskite layers and the above values of 10<sup>-4</sup> ÷ 10<sup>-2</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> in charge-transport layers (CTL) that the relation  $\mu_{\text{per}}/\mu_{\text{CTL}} \leq d_{\text{per}}/d_{\text{CTL}}$  is valid, where  $d_{\text{per}}$  and  $d_{\text{CTL}}$  are thicknesses of the perovskite layer and the CTL, respectively. This relation corresponds to the transport of charge carriers to electrodes without losses and delays at interfaces between functional layers.

*This work was supported by the Russian Science Foundation (project № 23-19-00884).*

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## Synthesis and Properties of Thiophene/Phenylene Co-Oligomers for Organic Electronics and Photonics

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Organic electronics are based on organic semiconductor materials. Among them, organic linear conjugated oligomers are of great interest for organic electronics and photonics as materials on the basis of which large-scale single crystals can be obtained by growth methods from solutions or from vapor. It should be noted that conjugated oligomers in organic electronics are individual compounds, since the classical mixture of oligomers with different numbers of repeating monomer units most often has mediocre semiconductor properties. This feature makes it possible to obtain ultrapure materials, which has a beneficial effect on their semiconductor and luminescent properties.

This report will present the features of the synthesis of conjugated oligomers based on phenyls and thiophenes. Various approaches and optimal conditions are demonstrated. It is shown how various synthetic schemes can lead to by-products of different structure, which can significantly affect the properties of the resulting materials.<sup>1</sup> Some structure-property patterns for thiophene-phenylene oligomers have been identified.<sup>2-7</sup> The introduction of 2,1,3-benzothiadiazole fragment into oligomers leads to significant changes in their properties. Benzothiadiazole is one of the most widely used acceptor moieties in low band gap materials for organic electronic applications. Motivation for incorporation of this heterocyclic unit into oligomers is its high absorption coefficient and luminescent quantum yield, large Stocks shift, low bandgap and excellent thermal stability. A large library of linear oligomers containing 2,1,3-benzothiadiazole fragment was synthesized.<sup>8-10</sup> The optical and thermal properties of the new compounds have been studied.

The presented organic conjugated oligomers can be used in various devices of organic photonics and electronics, such as organic field-effect transistors (OFETs)<sup>3,4</sup>, organic light-emitting transistors (OLETs)<sup>5,7</sup>, spectral shifting fibers<sup>11</sup>, liquid scintillators<sup>12</sup>, organic light-emitting diodes (OLEDs), CIGS photovoltaic devices<sup>13</sup>. Some oligomers are commercialized by a startup Limited Liability Company "Luminescent Innovative Technologies" (LumInnoTech LLC). All the details can be found on [www.luminnotech.com](http://www.luminnotech.com)

*This work was supported by Russian Science Foundation (grants № 22-13-00255).*

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## Expanding the Scope of Electrochemistry: Methods and Applications

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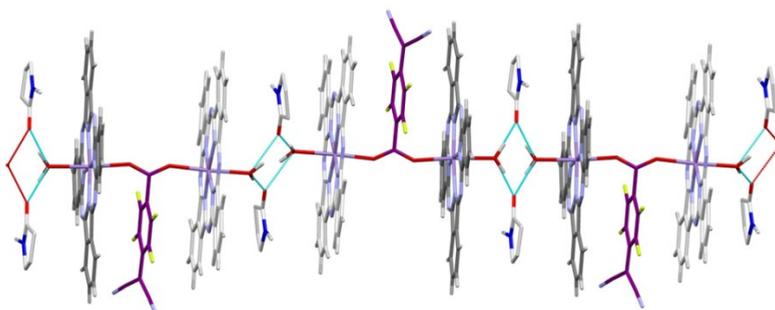
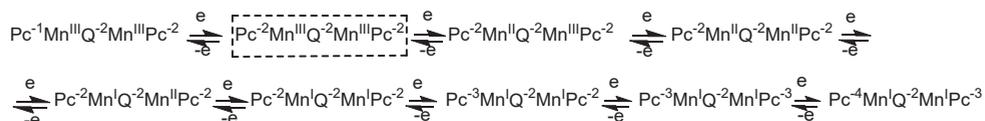
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The field of organic electrochemistry and electrocatalysis has seen significant advancements, broadening the potential applications and methods available for research and practical use. Although the primary focus lies within organic electrochemistry, materials pertinent to OLED technology and charge transfer complexes have also been explored, which are of great interest to the audience of this conference. Key topics include the principles and applications of electrochemistry, particularly in the context of organic compounds. The semi-differential method of cyclic voltammetry (CV) will be discussed, highlighting its utility in determining HOMO and LUMO energy levels. Attendees will learn what electrochemical measurements can reveal about a system, such as redox potentials and electron transfer rates, and what limitations exist in CV. The work aims to deepen the understanding of electrochemical techniques and their application in the study and development of advanced organic electronic materials.

This work will also cover fundamental principles and innovative techniques in organic electrochemistry, including the synthesis and characterization of novel organic compounds and their electrocatalytic properties. Additionally, the study examines strong acceptor molecules with polyaromatic ligands, their synthesis, electrochemical behavior, and applications in electronic devices.



Recent studies have demonstrated how the rational design of these complexes can lead to materials with desirable electronic properties. Methods for evaluating the size and properties of nanoparticles and quantum dots in the context of electrochemistry will also be discussed, which is crucial for the development of next-generation electronic materials.

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## Electron Spectroscopy Investigation of Energy Band Profiles of Conjugated Molecular Films on Semiconductor and on Metal Oxide Surfaces

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In this presentation a number of approaches to investigation of the energy position of the maxima of the valence band and of the conduction band of semiconductor organic materials is discussed, which can be carried out using photoelectron spectroscopy and total current electron spectroscopy. The possibilities of using these techniques to establish the height and extent of the interfacial potential barrier between an organic layer and an electrode material are considered. The results on a series of interface structures based on films of thiophene-phenylene co-oligomers, thienothiophenes and anthracenes, up to 10 nm thick, on the following substrates: SiO<sub>2</sub>, Au, CdS, ZnO, MoO<sub>3</sub> are presented. An important part of research should be devoted to characterization of the thin film and the ultra-thin film structures in order to prove reproducibility of the electronic properties of the structures investigated. Characterization techniques may include X-ray diffraction, atomic composition analysis (X-ray photoelectron spectroscopy), and surface topography analysis (atomic force microscopy).<sup>1</sup> Electronic properties of the surface organic layers can be tuned by means of the influence of the substrate material and by introducing polar substituents into the molecules.<sup>2</sup> Those changes may be readily monitored by the analysis of the density of valence states and of unoccupied electronic states (DOS and DOUS, respectively). Particular attention is paid to the techniques which use the low-energy electron beam as a probe of the materials under study, such as total current spectroscopy technique, electron attachment technique and to comparison of the experimental results with the results of the first-principle theoretical calculations.

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## ***n*-type Organic Ionic-electronic Mixed Conductors for Electronic Devices**

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Recently, conjugated polymers containing ethylene glycol-type side chains have emerged as a new class of organic mixed ionic-electronic conductors (OMIECs). This type of OMIEC is susceptible, stable in aqueous environments, and has a low working bias. They are also biologically and mechanically compatible with living tissues.<sup>1</sup> This makes organic electrochemical transistor (OECT) devices ideal for direct bioelectrical signal recording and stimulation when interfacing with active cells and tissues. OMIECs are miscible with dopant molecules and can be efficiently doped for thermoelectric devices, delivering high electrical conductivity and power factor.<sup>2</sup> Power-efficient complementary inverters/circuits and thermoelectric generators require both high-performance p-type and n-type OMIECs; however, developing n-type OMIECs lags much behind the p-type counterparts.

Here, we introduce molecular strategies, including side-chain engineering and backbone chemistry, to modulate the electronic and ionic charge transport properties of n-type OMIECs. For example, by customizing amphipathic side chains, the molecular packing of the conjugated polymer and the interaction with the dopant molecules or counterions can be optimized for better-mixed charge transport. Moreover, we tailored the molecular structures of a thiazole-flanked diketopyrrolopyrrole (DPP) based conjugated polymer through regio-chemistry and tuning the length of glycolated side chains. By doing so, we can improve charge transport through backbone chains by increasing the delocalization of charge carriers and altering the orientation of polymer chains, leading to better-coupled charge transport. By increasing the number of sp<sup>2</sup>-N substitutions, the density-of-state (DOS) profile can be tailored to switch the charge transport mechanism from a hopping transport to a coherent charge transport. Benefiting from these advanced molecular designs, we achieve an electrical conductivity of > 100 S cm<sup>-1</sup> and a figure-of-merit ZT of > 0.3 for n-type organic thermoelectrics and a figure-of-merit μC\* of > 100 F cm<sup>-1</sup> V<sup>-1</sup> s<sup>-1</sup> for n-type OECT devices.

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# Oral talks

## Template-Induced Crystallization of Novel Orthorhombic 9,10-Diphenylanthracene Polymorph

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Template-induced crystallization refers to the heterogeneous nucleation of a solute and is used to control polymorphism, crystal shape and size, and to obtain high-quality single crystals for X-ray structure determination<sup>1</sup>. The template component is introduced into the solution intentionally or it may appear naturally during the crystallization process.

Here, we studied template-induced crystallization of organic luminophore 9,10-diphenylanthracene (DPA) on the following crystals used as substrates: pyrene, perylene, anthracene, and rubrene. Crystallization of DPA in the presence of pyrene and perylene resulted in the formation of their co-crystals, whereas crystallization with anthracene and triclinic rubrene crystals had no effect on DPA polymorphism. Remarkably, the orthorhombic rubrene crystals promoted the crystallization of new orthorhombic DPA polymorph ( $\delta$ -DPA) on template crystals' side facets (Fig. 1a). Both template (orthorhombic rubrene) and  $\delta$ -DPA have the same orthorhombic crystal system with similar herringbone packing formed by C-H $\cdots\pi$  interactions, which induce epitaxial growth of the new phase (Fig. 1b). The growth of a new phase can easily be realized due to the formation of C-H $\cdots\pi$  interactions between DPA and RUB molecules within the layer with interaction energy of -40 kJ/mol (according to the values of this type of interaction). Phase analysis of DPA+Orth-RUB pattern shows the presence of small amount of  $\delta$ -DPA (Fig. 1c). In contrast,  $\delta$ -DPA and Tricl-RUB has different tilt of the DPA and rubrene molecules and in the latter the herringbone packing is absent; both factors may be the reasons for the lack of a template effect on Tricl-RUB for  $\delta$ -DPA crystal growth.

$\delta$ -DPA demonstrated a blue emission with photoluminescence quantum yield of 52% (Fig. 1d). This mimicry of the solute crystal structure to the template may be a powerful tool for crystal engineering of high-performance functional materials with desired optoelectronic properties.

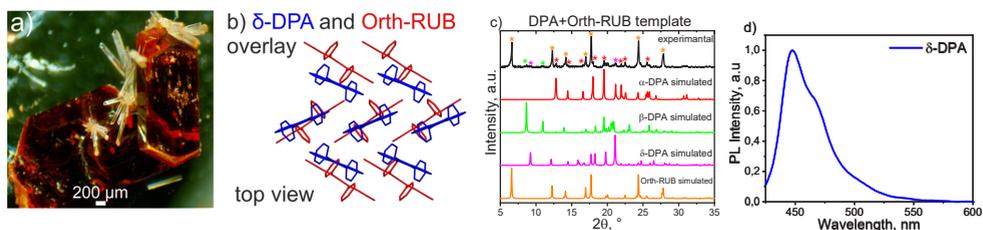


Fig. 1. Optical images of needle-like  $\delta$ -DPA crystals in the presence of red plate of Orth-RUB in reflected light (a);  $\delta$ -DPA and Orth-Rub herringbone packing overlay (b); powder X-ray diffraction data of DPA crystallized in the presence of the Orth-RUB (c); PL spectra of  $\delta$ -DPA crystals (d).

*This work was supported by RSF (project № 23-73-01263).*

## On the Influence of the Molecular Structure of Linear Thiophene-Phenylene Oligomers with a Central Benzothiadiazole Fragment on the Growth, Structure and Properties of Crystals

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*N.I. Sorokina*<sup>1</sup>, *O.V. Borshchev*<sup>2</sup>, *M.S. Skorotetsky*<sup>2</sup>, *E.A. Svidchenko*<sup>2</sup>, *N.M. Surin*<sup>2</sup>

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Linear thiophene-phenyl-benzothiadiazole oligomers with various groups of terminal substituents (Fig. 1) are highly stable luminophors with a large Stokes shift, the emission spectrum of which is in the range of 500 – 800 nm.<sup>1</sup> The physicochemical properties and crystallization nature of the compounds strongly depend on the order of the phenyl and thiophene groups in the structure of the conjugated nucleus, as well as on the presence of certain terminal substituent groups in the molecule. Studying the features of crystallization and crystal structure allows us to seriously deepen our understanding of the relationship between the molecular nature and properties of materials.<sup>2-3</sup> However, the currently available information on these compounds is still quite scarce and has not been systematized to establish structure-property relationships. The report will present the results of studies of growth from solutions, structure, thermal, electrical and absorption-fluorescent properties of crystals and solutions based on linear conjugated molecules with a central benzothiadiazole fragment and various combinations of thiophene and phenylene groups without terminal substituent groups and substituted with terminal trimethylsilyl groups (Fig. 1).

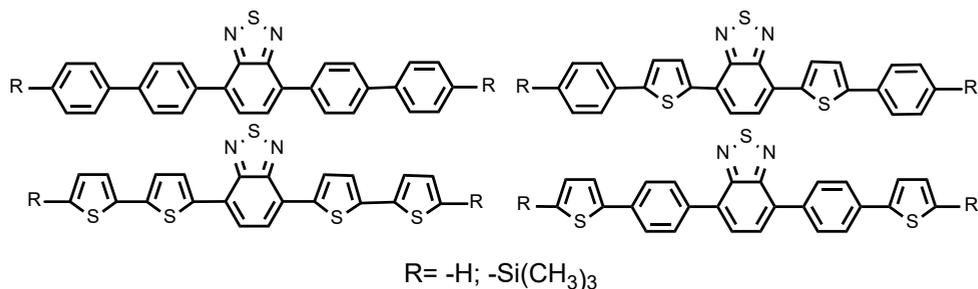


Fig. 1. Structural formulas of the studied oligomers.

*This work was supported by Russian Science Foundation (project № 22-13-00255).*

<sup>1</sup> M. S. Skorotetsky *et al.* *Dyes and Pigments*, 2018, 155, 284–291.

<sup>2</sup> V. A. Postnikov *et al.* *Crystals*, 2023, 13, 1697.

<sup>3</sup> V. A. Postnikov *et al.* *ACS Omega*, 2024, 9, 14932.

## Crystals of 4,7-di-2-Thienyl-2,1,3-Benzothiadiazole and its Derivatives with Terminal Trimethylsilyl and Alkyl Substituents: Synthesis, Growth, Structure, Electrical and Optical-Fluorescent Properties

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Among short donor–acceptor molecules with a central benzothiadiazole fragment, 4,7-di-2-thienyl-2,1,3-benzothiadiazole (T-BTD) attracts significant attention as a semiconductor compound with remarkable photophysical properties.<sup>1</sup> The addition of terminal substituent groups allows for the variation of the physicochemical characteristics of the compounds with the aim of enhancing thermo- and photostability and improving the physical properties of the crystals. This work is dedicated to the investigation of the growth, structure, thermal, electrical, and opto-luminescent properties of T-BTD crystals and its derivatives with terminal trimethylsilyl (TMS-T-BTD) and alkyl substituent groups (C6-, C8-, C10-, C12-T-BTD) (Fig. 1).

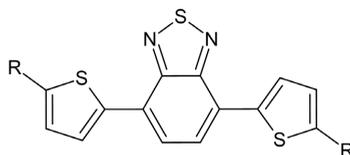


Fig. 1. General structural formula and abbreviations of the investigated oligomers:

R = -H (**2T-BTD**); -Si(CH<sub>3</sub>)<sub>3</sub> (**TMS-2T-BTD**); -C<sub>6</sub>H<sub>13</sub> (**C6-2T-BTD**);  
-C<sub>8</sub>H<sub>17</sub> (**C8-2T-BTD**); -C<sub>10</sub>H<sub>21</sub> (**C10-2T-BTD**); -C<sub>12</sub>H<sub>25</sub> (**C12-2T-BTD**)

The phase transition parameters and thermal stability of T-BTD and its derivatives were investigated using DSC and TGA methods. Single crystals of the synthesized compounds were grown from solutions. The crystal structure of T-BTD in the orthorhombic system (sp.gr. Pcab, Z=8) was refined by single-crystal XRD analysis, and for the studied derivatives, the crystal structures were determined for the first time: in the monoclinic system for TMS-T-BTD (sp.gr. P2<sub>1</sub>/c, Z=4) and C6-T-BTD (sp.gr. P2<sub>1</sub>/n, Z=4), and in the triclinic system for C8-, C10-, and C12-T-BTD (sp.gr. P-1, Z=2). The relationship between observed growth anisotropy and molecular packing in the crystals was analyzed. Intermolecular interactions in the crystals of the studied compounds were modeled using Hirshfeld surface analysis. The spectral-fluorescent properties of the compounds in crystalline films and solutions were studied. The solvatochromic effect for T-BTD and TMS-T-BTD was studied in various solvents (*n*-hexane, THF, dichloromethane, and acetonitrile), and the photostability in *n*-hexane solutions was investigated.<sup>2</sup> The electrical properties of thin polycrystalline films, deposited via vacuum thermal evaporation, were studied using the field-effect transistor method.

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

<sup>1</sup> A. Iagatti et. al. *Phys. Chem. Chem. Phys.* 2017, **19**, 13604.

<sup>2</sup> V.A. Postnikov et. al. *Crystals*, 2023, **13**, 1697.

## The Impact of ZnO Surface on the Stability of Perovskite Films and Solar Cells

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Herein, we present a comparative study of different solution-based and solution-free zinc oxide deposition methods in the context of their impact on the stability of ZnO/perovskite interface using a series of complementary experimental and computational methods. Thus, it has been revealed that the OH-terminated oxide surface induced severe degradation of all types of perovskite absorbers. The zinc oxide passivated from the surface with acetate groups was found to be very aggressive toward MAPbI<sub>3</sub> and quite inert with respect to a methylammonium-free perovskite formulation. Most notably, the amine-passivated ZnO films induced no degradation of the perovskite absorber films, whereas the corresponding perovskite solar cells retained 70% of the initial efficiency after 2500 h of continuous operation under open circuit conditions and white light irradiation, which is an impressive result for devices with n-i-p geometry. Thus, the presented results demonstrate the power of the surface chemistry that can alter completely the behavior of the ZnO films; this approach holds a great potential for tailoring the properties of other oxide materials such as TiO<sub>2</sub>, SnO<sub>2</sub>, NiO, etc. to pave a way to efficient and stable perovskite solar cells.

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## Towards Adaptation of the Industrial Requirements for Up-Scaling of Perovskite Solar Modules

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Fig. 1. Foldable Perovskite Solar Panel fabricated in NUST MISIS

Perovskite solar modules are on the way towards passing the standard tests of terrestrial solar cells accord to the requirements of stability and prototype geometry. Among the other strategies to mitigate the common corrosion issues in up-scaled perovskite solar modules, the interface passivation was considered as efficient strategy.

In this research, we are demonstrating the experience for prototyping of perovskite solar modules and panels with advanced interface engineering using approaches of surface modification in absorbers, integration of self-assembling monolayers in charge transport junctions. We analyzed the state-of-the-art in stabilization of perovskite solar panels by industrial leaders and academic community. The critical issues in solution – processing cycle as well as high-throughput production were identified.

The specific cases of slot-die coating, laser-scribing, multi-layer passivation, uniform photo-response for perovskite solar modules of high PCE (>15%) and lifespan (over 1500 h) were discussed. We found that standard charge transporting layer, as well as multi-cation perovskites requires advanced surface modification to prevent electrochemical corrosion induced by intrinsically formed ionic defects.

*This work was supported by Priority2030 program of NUST MISIS with Grant K2-2022-011.*

## New Non-Fused Asymmetric Nonfullerene Acceptors for Polymer Solar Cells

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Here in, we have designed two new unfused non-fullerene small molecules based on asymmetric benzo[1,2-b:3.4-b', 6,5-b"]trithiophene (BTT) central donor core and different terminal units, i.e. 2-(3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (NFA-4) and 1,3-diethyl-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (NFA-5) and their optical and electrochemical properties were investigated. Employing a wide bandgap copolymer D18, the binary D18: NFA-4 and D18:NFA-5 bulk heterojunction-based organic solar cells realized an overall power conversion efficiency of about 17.07% and 11.27 %, respectively. The higher value of power conversion efficiency for the NFA-4-based organic solar cells, as compared to the NFA-5 counterpart, is attributed to the enhanced values of short circuit current, open circuit voltage, and fill factor. After the incorporation of NFA-5 into the binary bulk heterojunction D18:NFA-4, the ternary organic solar cells attained a power conversion efficiency of 18.05 %, which is higher than that for the binary counterparts and attributed to the increased values of short circuit current, fill factor, and open circuit voltage. The increased value of short circuit current is associated with the effective utilization of excitons through the energy transfer from the NFA-5 to NFA-4 as the NFA-4 exhibits a more significant dipole moment than the NFA-5 and is effectively dissociated into a free charge carrier.

*This work was supported by RSF 124-43-00178*

## Self-Assembled Monolayer Materials Based on Triphenylamine with Anchor Groups for Perovskite Solar Cells

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Among the various emerging areas of organic photovoltaics, perovskite solar cells (PSCs) stand out as a particularly promising field, with these devices demonstrating the potential to achieve remarkable efficiency levels exceeding 26%.<sup>1</sup> A significant aspect of PSCs is the incorporation of intermediate interface layers, specifically hole-transport (HTLs) and electron-transport (ETLs), which facilitate effective charge transport from the active layer of the perovskite to the electrodes. This not only enhances the device's performance but also minimises energy losses by establishing a seamless energy transition between the active layer and the electrode. Furthermore, in a p-i-n structure, the HTL plays a crucial role in enhancing the device's stability by effectively suppressing the mobility of ionic defects and reducing the concentration of traps.<sup>2</sup> It is therefore imperative that researchers prioritize the development of new SAM materials.

In this study, three new semiconductor materials, TPATC, TPABC and F-TPATC, were synthesised. These are based on triphenylamine with various substituents (hydrogen or fluorine), as well as with various spacer fragments (thiophene or benzothiadiazole). In the context of PSCs, a carboxyl group conjugated with the triphenylamine fragment through a spacer bridge was employed as an anchor group, with the objective of establishing a potentially superior contact surface with the electrode or perovskite material. The optical, thermal and electrochemical properties of the molecules, the hydrophobicity of the resulting surface and the influence of these properties on the photovoltaic parameters of devices were studied and compared. The materials were tested as hole-transporting materials in PSCs, which exhibited high efficiency values exceeding 20%, as well as excellent stability. For TPATC, the loss in efficiency did not exceed 5% over 1000 hours. Furthermore, TPATS was tested in a perovskite solar module with an active area of 64 cm<sup>2</sup>.

*This work was supported by Russian Science Foundation as part of grant No. 22-19-00812.*

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<sup>1</sup> Devadiga D. et al., *International Journal of Energy Research*, 2021, **45**(5), 6584–6643.

<sup>2</sup> Pham H.D. et al., *Advanced Energy Materials*. 2020, **10**(13), 1903326.

## Multiscale Quantum Chemical Calculations of Highly Efficient Narrowband Deep-Blue Fluorophores

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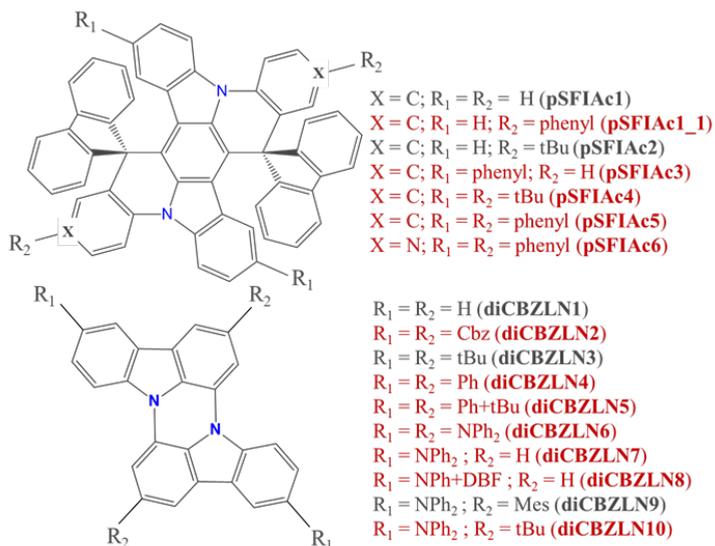


Fig. 1. Structures of studied pSFIAC and diCBZLN derivatives

In this work the spectral properties of pSFIAC and diCBZLN based deep-blue luminophores is studied taking into account their environment. The structures of the dopants with different hosts were generated using molecular dynamics. The fluorescence spectra of the dopants with hosts were calculated using TD-DFT method. The environment of the chromophores was modelled as a QM/MM approach, and as effective fragment potentials (EFP) method. It was found that the use of a multiscale approach allows one to increase the accuracy of the results obtained, without using computationally expensive functionals, and also to accurately predict the shape of spectral lines without calculating vibration frequencies.

*This work was supported by the Ministry of Science and Higher Education within the State assignment (project № FFSM–2022–0004) in part of QM calculations and by RSF (project № 23-23-00429) in part of MD, QM/MM and QM/EFP calculations.*

## Geminate Recombination Kinetics in Organic Semiconductors, Controlled by Extremely Non-Equilibrium Hopping Transport

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Photogeneration and transport of charge carriers (electrons and holes) are the key physical processes that underlie the operation of photovoltaic devices based on disordered organic semiconductors. Since the dielectric constant of organic semiconductors is small, the electron and hole remain connected by the Coulomb interaction after the decay of a molecular exciton on the spatial scale of the Coulomb radius, which is much larger than the typical hopping length. A geminate pair arises, the probability of separation of which determines the efficiency of photogeneration. Hopping drift and diffusion of “hot” geminates over a significant time interval, due to disorder, occur in an extremely nonequilibrium (dispersive) regime. The effect of disorder on the carrier photogeneration efficiency is undoubtedly significant. It has long been shown experimentally, by the Monte Carlo method<sup>1</sup> and, recently, analytically<sup>2,3</sup> that the separation probability of a pair at low temperatures is much greater than predicted by the classical Onsager model, and it weakly depends on the field strength. This is in part caused by anomalously strong diffusion at short times, when (in the regime of jumps down in energy) the Einstein relation is violated, and in part by the presence of an electric field, which cannot be considered weak at low temperatures. A simple analytical expression is derived that includes the calculated effective initial pair separation and the effective (field dependent) temperature<sup>3</sup>, in good agreement with Monte-Carlo<sup>1</sup> and experimental<sup>4</sup> data.

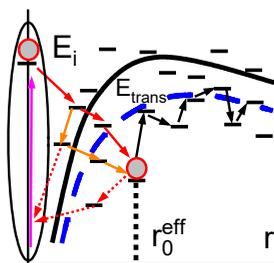


Fig. 1. Scheme of the separation of the geminate pair.

An alternative to geminate pair separation is geminate recombination. In this work, we calculated the time dependences of the survival probability and the rate of geminate recombination. The latter determines the intensity of photoluminescence. The applicability of this model to various organic materials is discussed.

*This work was supported by Russian Science Foundation, project 22-22-00612.*

<sup>1</sup>Albrecht U., Bäessler H. Chem. Phys. Lett. 1995, 235, 389–393.

<sup>2</sup>Toropin A.V., et al. J. Phys. Chem. Lett. 2023, 14, 7892–7896.

<sup>3</sup>Toropin A. V., et al. J. Phys. Chem. Lett. 2024, 15, 3884–3892.

<sup>4</sup>Im C., et al. J. Chem. Phys. 2002, 117, 2961–2967.

## Analytical Modeling of Hopping Transport of Charge Carriers and Excitations in Materials with Correlated Disorder

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Spatial-energy correlations strongly influence charge and exciton transport in weakly ordered media, such as organic semiconductors and nanoparticle assemblies. We develop a unified analytic approach for calculating temperature and field dependence of charge carrier mobility in organic quadrupole glasses and temperature dependence of the diffusion coefficient of excitons in quantum dot solids<sup>1</sup>. We obtain analytic expressions for the energy distribution of hopping centers, the characteristic escape time of charge/exciton from the energy well stemming from energy correlations around deep states, and the size of the well using the approach initially developed for the charge transport in organic dipole glass<sup>2</sup>. The derived formulas are tested with Monte Carlo (MC) simulation results<sup>3</sup>, showing good agreement, and providing simple analytic expressions for analysis of charge and exciton mobility in a broad range of partially ordered media. The results are presented on Fig.1a (temperature dependence of diffusion coefficient of triplet excitons in quantum dot solids and charge transport in organic quadrupole glasses) and Fig.1b (field dependence of charge carrier mobility in quadrupole glasses).

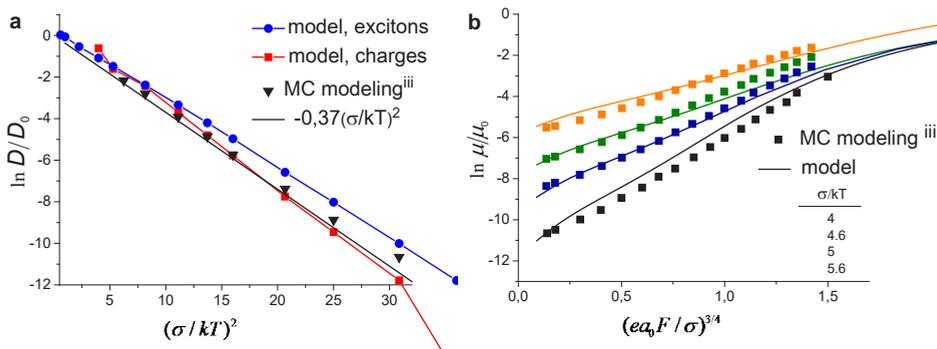


Fig. 1. Calculation results in comparison with MC simulation data<sup>iii</sup>.

*This work was supported by RSF (project № 22-22-00612).*

<sup>1</sup> Saunina A. Yu., Libai H., Nikitenko V. R., Prezhdo O.V., *J. Phys. Chem. Lett.* 2024, **15**(9), 2601.

<sup>2</sup> Nikitenko V. R., Saunina A. Yu., Tyutnev A. P., Prezhdo O.V., *J. Phys. Chem. C* 2017, **121**(14), 7776.

<sup>3</sup> Novikov S. V., Vannikov A. V., *J. Phys. Chem. C* 2009, **113**, 2532.

## Impact of Electronegative Atoms on Dynamic Disorder in Crystalline BTBT Derivatives

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The use of organic semiconductors (OSs) in high-performance organic electronic devices requires a high mobility of charge carriers in them. Among the main factors determining the charge-carrier mobility in high-mobility OSs is the dynamic disorder – fluctuation of the positions and relative orientations of molecules induced by thermally activated low-frequency (LF, wavenumbers below 200 cm<sup>-1</sup>) vibrations. This disorder results in the variance of transfer integrals, which disrupts intermolecular charge delocalization and hinders efficient coherent charge transport. Thus, suppression of dynamic disorder is highly desirable for increase of charge-carrier mobility, and formulation of the relationship between molecular/crystal structure and dynamic disorder is of great importance.

In this study, we address the effect of electronegative atoms – fluorine and nitrogen – on dynamic disorder in high-mobility diphenyl-substituted derivative of [1]benzothieno[3,2-b][1]benzothiophene (BTBT), Ph-BTBT. Four compounds – mPy-BTBT and pPy-BTBT with one nitrogen atom per phenyl ring, FPh-BTBT with one fluorine atom per phenyl ring, and F<sub>5</sub>Ph-BTBT with perfluorinated phenyl rings – were synthesized; the latter two compounds are novel. We observed that relative LF intensity of experimental Raman spectra (quantified by *R* descriptor), which can be used as an experimental estimate of dynamic disorder,<sup>1</sup> is lower for compounds with one fluorine or nitrogen atom per phenyl ring than for non-substituted Ph-BTBT, but is much higher for F<sub>5</sub>Ph-BTBT (see Fig. 1). In line with this finding, our calculations based on solid-state DFT showed the similar trend in the variance of transfer integrals, highlighting that electronegative atoms can facilitate suppression of dynamic disorder. The observed effect of the electronegative atoms on dynamic disorder is explained by their impact on intermolecular interactions.<sup>2</sup> The results obtained provide guidelines for design of OSs with suppressed dynamic disorder and hence potentially high charge mobility.

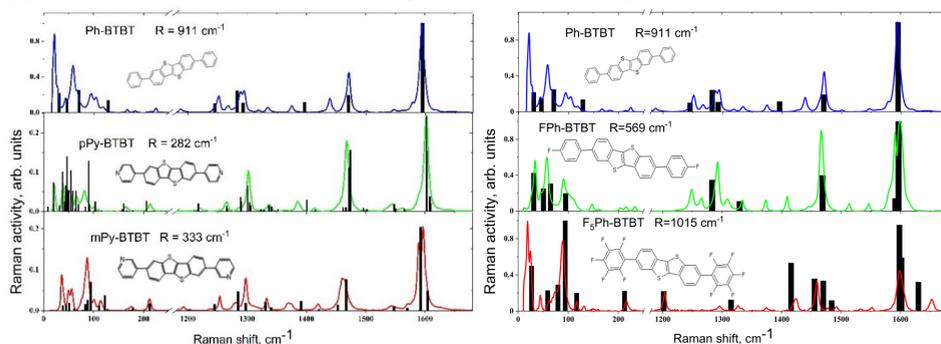


Fig. 1. The impact of nitrogen (left) and fluorine (right) substitution on experimental (lines) and calculated (bars) Raman spectra the compounds studied.

*The study was supported by Russian Science Foundation (Project #22-72-10056).*

<sup>1</sup> M.V. Vener et al., *Adv. Electron. Mater.* **7**, 2001281, 2021.

<sup>2</sup> A. Yu. Sosorev et al., *Phys. Chem. Chem. Phys.* **23**, 15485-15491, 2021.

## Electronic Nose Based on Siloxane Derivatives of BTBT with Different Length of Terminal Alkyl Groups

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The monitoring and quantitative analysis of various gas mixtures are becoming increasingly important and relevant, both from safety and personalized medicine points of view. These monitoring tasks may include the analysis of ambient air, analysis of food freshness, diagnostics of diseases by analyzing exhaled air, etc. Thin-film organic field-effect transistors (OFETs) are promising sensor devices for detecting low concentrations of various gases due to their high sensitivity at room temperature, low power consumption, and flexible architecture. Such high sensitivity is achieved due to the direct interaction between the thin conducting layer of the OFET and the substance being analyzed.<sup>1</sup> Previously published works demonstrated that benzothienobenzothiophene (BTBT) siloxane dimer molecules are successfully used in such devices as OFETs,<sup>2</sup> chemosensors,<sup>3</sup> and an electronic noses.<sup>4</sup> Usually, different receptor layers are used to vary the sensitivity and selectivity of such devices, while only a few works are devoted to an electronic nose based on OFETs made of various organic semiconductors.<sup>5</sup> It should be noted that the latter approach has some advantages, since it does not require the manufacture of additional receptor layers that can damage the semiconductor layer of the OFET.

In this work, the effect of the terminal alkyl group length (from zero to thirteen carbon atoms) of BTBT siloxane dimers on the electrical and sensory properties of OFETs based on them was investigated using various target analytes (ammonia, hydrogen sulfide, nitrogen and sulfur dioxides). The studied devices exhibited a behavior typical of p-channel devices, and the calculated values of charge carrier mobility, threshold voltages and on-off current ratios were  $10^{-5}$ – $10^{-2}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>, from -24 to +14 V and  $10^2$ – $10^7$ , respectively. As for the sensory properties, the devices demonstrated a clear difference in sensitivity and selectivity depending on the target analyte and the dimer used. From the fundamental point of view, this investigation allows to shed some light on the mechanism of sensory response for such devices. For practical application it opens the way to the creation of an electronic nose based on OFETs from different organic semiconductors, the chemical structure of which does not change much, which makes it possible to form layers under almost identical conditions.

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

<sup>1</sup> A. A. Trul et al., *J Mater Chem C*, 2018, **6**, 9649-9659.

<sup>2</sup> A. S. Sizov et al., *ACS Appl Mater Interfaces*, 2018, **10**, 43831–43841.

<sup>3</sup> A. A. Trul et al., *Sens Actuators B-Chem*, 2020, **321**, 128609.

<sup>4</sup> D.S. Anisimov et al. *Sci Rep*, 2021, **11**, 10683.

<sup>5</sup> J.B.Chang et al. *Journal of Applied Physics*, 2006, **100** (1).

## A Close Look at Dielectric Elastomer Actuators

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Artificial muscles are soft actuators capable of generating force and shape change in response to external stimuli, such as pH, temperature, humidity, and electric and magnetic fields. The force and strain generated by most soft actuators are too small to be used as artificial muscles. The most promising technology closely emulating natural muscles is dielectric elastomer actuators (DEA). They are soft capacitors that deform when electrically charged and recover the initial shape when discharged due to the elastic restoring forces. In addition to general requirements – reliability, compactness, durability, adaptability, etc. – the DEAs should be operable at low voltages. However, existing DEAs do not meet the safety standard for such applications because of the high driven voltages.

Pelrine's model suggests two ways to achieve high thickness strain ( $s_z$ ) at low voltages ( $V$ ): increase the ratio between the relative dielectric constant ( $\epsilon$ ) and the Young's modulus ( $Y$ ), and decrease the DE film thickness ( $z$ ):

$$s_z = -\epsilon_0 \frac{\epsilon}{Y} \left(\frac{V}{z}\right)^2$$

$\epsilon_0$  is the free-space permittivity ( $8.85 \times 10^{-12} \text{ F m}^{-1}$ ) in Eq. 1.

Here we will discuss the classes of commonly used DE materials, and highlight the main approaches to lower the  $\epsilon/Y$ . We used circular DEA (cDEA), which was prepared by equibiaxial stretching of the DE film followed by the electrode deposition. We a cDEA configuration active area of which can expand reversibly under applied electric field (Fig. 1a), as well as a cDEA design that can bear a load and displace it under the applied electric field. The first results of this work will be presented at the meeting.

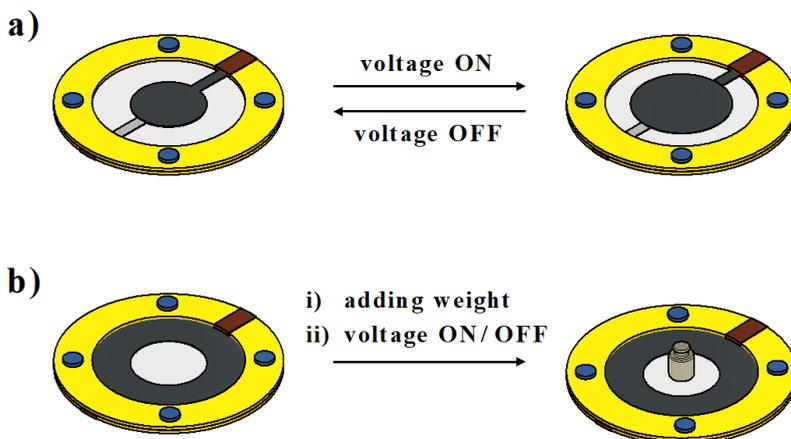


Fig. 1. Two designs of circular dielectric elastomer actuators (cDEA) used in this study. (a) The active area of the cDEA reversibly expands under applied electric field; (b) the cDEA displaces the load when electric field is applied.

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## Intermolecular Interaction Energy-Based Computational Screening of High-Mobility Organic Semiconductors

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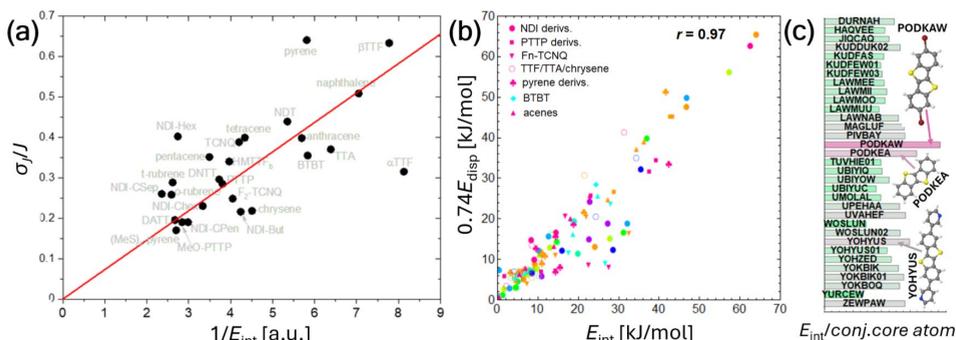


Fig. 1. (a) Correlation of the inverse intermolecular interaction energy  $1/E_{\text{int}}$  and relative variance of transfer integrals measuring the dynamic disorder in representative crystalline organic semiconductors; (b)  $E_{\text{int}}$  versus the Grimm's dispersion correction; (c) selected structures revealed using a fast  $E_{\text{int}}$ -based screening of the Cambridge Structural Database.

Further progress in organic electronics critically depends on efficient discovery of novel organic semiconducting materials, notably including high-mobility crystalline semiconductors. However, despite a variety of currently known crystals formed by conjugated organic molecules, only few of them have structures with a low dynamic disorder, a key ingredient to guarantee a high intrinsic charge-carrier mobility. Because of that, a computational search for the promising structures based on a blind, physics-unaware feature engineering becomes inefficient. In contrast, in our work, we develop a computational screening methodology based on physically transparent descriptors related to the crystal rigidity, such as the intermolecular interaction energy  $E_{\text{int}}$ . In particular, we demonstrate a promising correlation between the dynamic disorder and the inverse interaction energy,<sup>1</sup> whereas the latter turns out to correlate well with the dispersion term in it (Fig. 1a,b). Furthermore, various approximations are admissible here, e.g., the numerically straightforward atomistic Grimm's dispersion correction or the  $E_{\text{int}}$  estimation using a DFT-based Bader analysis.<sup>2</sup> On the practical side of the issue, using these correlations, we carry out a screening of a structural database, revealing low-disorder organic crystals (Fig. 1c) that could potentially be used in high-performance organic semiconducting devices. This conclusion is additionally justified by the charge-carrier mobility calculations. We thus expect that our computational screening methodology can facilitate discovery of new high-mobility organic semiconducting materials.

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

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<sup>2</sup> Sosorev A.Yu. et al., *J. Phys. Chem. C* 2023, **127**, 17948–17957.

## Towards the High Shelf Life Stability of BTBT Semiconductor Materials

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Organic semiconductor materials based on benzothieno[3,2-b][1]benzothiophene (BTBT) are widely used to create various types of organic field-effect transistors, such as thin film transistors, phototransistors, and electrolyte-gated transistors.<sup>1</sup> The advantage of BTBT materials is the high crystallinity, which allows achieving high charge carrier mobility.

The most common BTBT-based material is 2,7-dioctyl-BTBT, which has been used to achieve record charge carrier mobility. However, films based on small BTBT molecules are characterized by instability and a transition from the thin film phase to the bulk phase, which leads to a significant change in morphology and, therefore, electrical characteristics.<sup>2,3</sup> Therefore, in this work we will consider different approaches to overcome the problem of morphological instability of BTBT-based materials through molecular design.

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

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## The Design of Bio-Recognizing Surfaces for Application in Sensors for Fungal Pathogen Detection

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Invasive mycoses present a serious threat to public health, particularly for individuals with immunosuppression. The prevalence of these infections has significantly increased in recent years. According to estimates, the annual incidence of invasive fungal infections in 2024 is expected to be 6.5 million cases, resulting in approximately 3.8 million deaths. Of these deaths, about 2.5 million are directly attributed to fungal infection<sup>1</sup>.

Despite the urgent need for early detection of fungal infections, currently, there are only limited options available. This stimulates the development of highly sensitive sensors that can detect specific fungal markers at extremely low concentrations. In addition to the traditional ELISA (enzyme-linked immunosorbent assay) and LFT (lateral flow test) tests, we consider diagnostic platforms that are based on innovative nanophotonic<sup>2</sup> and electrochemistry<sup>3</sup> principles which require the creation of various types of bio-recognizing surfaces. Recent advances in regio- and stereoselective synthesis of oligosaccharide ligands related to fungal antigens<sup>4</sup> made it possible to develop such products.

In this communication we consider different methods for immobilization of bio-recognizing molecules (such as antibodies and antigens) onto the surface of gold nanoparticles, magnetic microparticles, dielectric and electrochemical surfaces. The density, equimolarity and controllability of presentation on the surface play an extremely important role for assaying results<sup>5</sup>. Special attention is paid to the stability of the surface after modification and to the control of its binding activity. These results have important methodological implications for the development of sensors based on various technological platforms that can be used to detect fungal markers.

*This work was supported by the Ministry of Science and Higher Education of the Russian Federation (agreement no. 075-03-2024-401/3 from 30.05.2024).*

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## Universal Approach to Fabrication of Reusable EGOFET Aptasensors Based on Track Membranes

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Biosensors based on electrolyte-gated organic field-effect transistors (EGOFET) are very promising devices for biological research and clinical diagnostics due to their inherent advantages, such as cost-effectiveness in use and sensitivity for different analytes. However, they also have some disadvantages. One of the main problems is the difficulty or impossibility of reusing the device. Even in cases where it is possible to restore the biorecognition layer, this is associated with labor-intensive procedures that often lead to a decrease in sensitivity.

Often, the biosensitivity of EGOFET is realized by modifying the gate or surface of the organic semiconductor (OS) of the transistor. In this paper, a new approach to creating a receptor layer in the composition of an EGOFET-based aptasensor using track membranes is proposed. The membrane is located on the OS surface, acting as a bioreceptor layer due to modification with a DNA aptamer.

- The detection limit of this sensor is  $1 \cdot 10^5$  VP/mL, which is superior to antibody-based rapid analysis test systems ( $1 \cdot 10^6$ - $4 \cdot 10^8$  VP/mL), but inferior to the PCR method ( $3 \cdot 10^2$ - $1.2 \cdot 10^3$  VP/mL);
- This approach opens up the possibility of creating a reusable biosensor, which was not possible in the case of modification of the semiconductor directly with a receptor layer.

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## Engineering Performance of High-Frequency Organic Electronic Devices

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Considering the increased popularity of the Internet of Things (IoT) and Wireless Sensor Networks (WSN), RF energy harvesting (WEH) is in demand. Because it will be able to recharge and even, in some cases, replace batteries. That would make the life span of these devices longer, easier to maintain and reduce power wastage. It will also facilitate lightweight wearable devices a reality. The electromagnetic spectrum in 30GHz~3THz range is attracting attention for potential applications in hidden weapon detection, aviation assistance, and spectroscopy for detecting harmful molecules and breath analyses, short-range radar, secured high-speed data transmission and more.<sup>1</sup> A critical component for the electronic circuitry for these applications is a detector, i.e., a rectifier. A sufficiently large communication range is essential for WEH applications. Since the path loss of an EM-far-field strength is inversely proportional to the square of the distance, the threshold voltage of the diodes must be as small as possible. Hence, there is a need for a Schottky barrier diode (SBD), which satisfies these requirements, and they are termed as ‘super-rectifiers’. This device has threshold voltages less than 0.2V. Despite of limited charge carrier mobility, organic semiconductors have potential to be implemented in these applications. We will demonstrate experimental device fabrication and measurement methods to realize this technology.<sup>2</sup> The planer SBDs are fabricated using molecular adhesion lithography with channel length of ~15 nm. Organic molecular or polymeric semiconductors are deposited by solution or evaporation. The devices are able to rectify the RF signals > 100 GHz with DC output power in  $\mu$ W to mW.<sup>3</sup> Further, integration of these high-speed rectifiers in the circuit should be accompanied by matching field-effect transistors. We will briefly discuss prospects of enhancing operation speeds of OFETs.<sup>4,5</sup>

*This work was supported by SERB India and Alexander von Humboldt Foundation Germany.*

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## The Design and Application of Organic Room-Temperature Phosphorescent Materials

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Room-temperature phosphorescence (RTP) is a phenomenon where excitons typically radiate from the lowest excited triplet state. The efficient generation, controllable management, and on-demand migration of triplet excitons in organic molecules have combined to constitute the long-sought Holy Grail of efficient RTP. Achieving this goal hinges on improving intersystem crossing (ISC) and suppressing the triplet nonradiative processes. The El-Sayed's rule has been recognized as an effective strategy for promoting ISC. Our work is centered around regulation of the coupling between different excited triplet states to enable multiple phosphorescence emission, thereby increasing triplet exciton utilization efficiency. We proposed that through-space charge separation between electron donor and acceptor is an effective strategy for triggering multiple phosphorescence,<sup>1,2</sup> elucidating that the decoupling between different excited triplet states is fundamental to this emission.<sup>3</sup> Finally, we demonstrated the utility of emitters with multiple phosphorescence in organic light-emitting diodes.<sup>4</sup> These findings highlight the potential of RTP materials to explore new structural spaces for optoelectronic materials, advancing modern device technology and engineering.

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# Poster presentations

## Synthesis and Properties of New BTBT Derivatives for Organic Electronics

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The research of new molecules and their properties plays a crucial role in various fields of modern science and technology. Over the past decade, thienothiophenes have become an excellent foundation for the development of hole-transport materials for organic electronics.<sup>1</sup> However, the derivatives of donor-acceptor type materials (D-A materials) with various nitrogen-containing moieties and their electron transport characteristics remain largely unexplored. Therefore, the synthesis and investigation of structures based on D-A materials and various nitrogen-containing precursors is a necessary part of the search for materials with optimal optoelectronic properties.

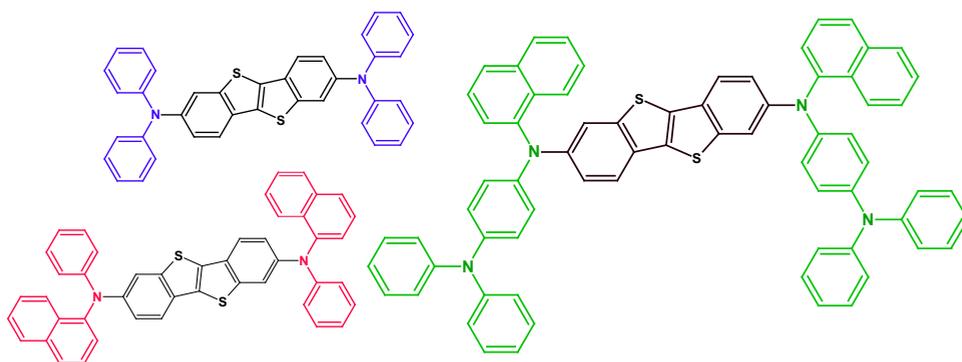


Fig. 1. Structures of new BTBT derivatives

The objective of this study is the synthesis of new structures, presented in Figure 1, based on BTBT (Benzothieno[3,2-b][1]benzothiofene) derivatives, and the investigation of their optical and thermal properties. The previously obtained dibromo-BTBT derivative was subjected to Buchwald-Hartwig coupling reactions with various amines. The obtained compounds were purified using flash chromatography and recrystallization, and their structure was established and confirmed by modern analytical methods. It is shown that with the complication of the amine fragment, the quantum yield significantly decreases from a satisfactory 60% to an extremely low 16% and the drain shift increases from 20 to 90 nm. The thermal properties of the obtained materials are comparable or exceed those of commercially demanded NPB.<sup>2</sup> This provides prospects for further research. We believe that derivatives can also work well in TADF OLED, OPV, PLED and QLED systems, providing their outstanding stability and resolution.

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

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## Synthesis and Aggregation-Induced Emission of 1,4-Bis((9*H*-Diazafluoren-9-ylidene)Methyl)Phenylenes

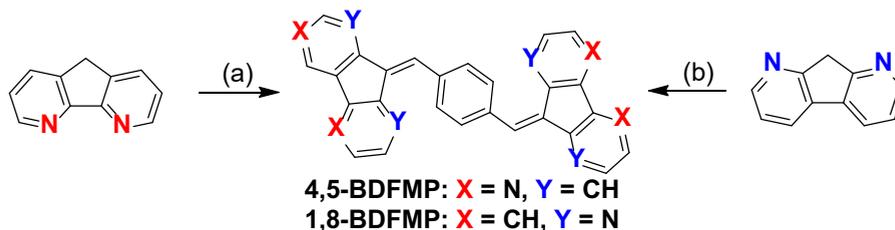
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Aggregation-induced emission (AIE)<sup>1</sup> materials are widely used as functional layers in organic light-emitting diodes, in bioimaging and medical science because they may provide high emission efficiency, high contrast, and stimuli response. AIE-active materials were also extensively used in sensorics as chemo-, mechano- and bio-probes. Some fluorenylidene derivatives possess aggregation-induced emission and are of a certain interest in organic electronics due to their high conformational lability, one-rotor structure, and sensitivity to external stimuli.<sup>2</sup> Replacing the carbon atoms in the fluorene moiety with a nitrogen atom at the 1,8-positions may result in high planarity and rigidity. At the same time, the introduction of nitrogen at the 4,5-position of the fluorene moiety may lead to complexing abilities and sensory properties.<sup>3</sup>

Here we present the synthesis of 1,4-bis((9*H*-diazfluoren-9-ylidene)methyl)phenylenes, which were obtained by condensation reactions of 1,8- and 4,5-diazfluorenes with terephthalic aldehyde (Figure 1). Both compounds were shown to have aggregation-induced emission. The photoluminescence quantum yield in solution was lower than 0.1%, while in the crystalline state the photoluminescence quantum yield is 10% for the 1,8-diazfluorene derivative and up to 25% for the 4,5-diazfluorenylidene derivative. The position of nitrogen atoms and its effect on the diazfluorene reactivity, crystal packing, molecular rigidity and planarity are discussed.



**Fig. 1.** Synthesis of 1,4-bis((9*H*-diazfluoren-9-ylidene)methyl)phenylenes. (a) terephthalaldehyde, TiCl<sub>4</sub>, Py, THF, 50°C, 72h; (b) terephthalaldehyde, NH<sub>4</sub>OAc, HOAc, 100°C, 12h.

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

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## Synthesis of Conjugated Polymers Based on Triphenylamine for Application in Perovskite Solar Cells and Metal-Ion Batteries

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Currently, a wide range of organic hole-transport materials used in perovskite solar cells is known.<sup>1</sup> Among them, due to the presence of such properties as high thermal stability, good solubility in organic solvents, improved adhesion to the substrate, high solution viscosity, good film-forming ability, special attention is paid to polymers based on triphenylamine derivatives (TPA). The high viscosity of the solution and good film-forming ability contribute to the production of homogeneous films, which has a beneficial effect on the crystallization of perovskite deposited on the polymer.

Another application of TPA-based polymers is their use as organic electrodes in metal-ion batteries. Thanks to TPA polymers, it is possible to create a system with high resistance to oxidation in air and a large surface area, which leads to high capacitive characteristics of devices.<sup>2,3</sup>

Among such materials, one of the most promising are donor-acceptor (D-A) polymers.<sup>4</sup> By changing the structure of the side chains of polymers by introducing various electron-acceptor groups, it is possible to effectively regulate the optoelectronic properties of materials: the region of light absorption, the energy of the HOMO and LUMO levels, charge mobility, which in turn can improve the output parameters of organic perovskite solar cells.

One of the widely used methods for the synthesis of TPA-based polymers is oxidative polymerization with FeCl<sub>3</sub>. This method is simple and does not require the use of expensive catalysts and toxic organoelement compounds.<sup>4,5</sup>

This paper presents polymers based on TPA D-A structure obtained by oxidative polymerization. Their optical, electrochemical, and thermal properties have been studied. The results obtained from studying materials in perovskite solar cells as a hole-transport layer are presented. It is shown how the introduction of polymer HTL improves the surface of the substrate and promotes better crystal growth. Primary data on the study of the polymer as a cathode material in sodium-ion batteries are also presented. The use of TPA polymer resulted in stable devices with high voltage.

*This work was supported by the Ministry of Science and Higher Education of the Russian Federation (agreement № 075-15-2024-532-2 under grant № 075-15-2024-532).*

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## Tuning Molecular Packing and Charge Transport in Thiophene-Phenylene Co-Oligomer Single Crystals for Field-Effect Devices

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Organic semiconductors combining efficient charge transport and bright luminescence are promising materials for organic optoelectronic devices. However, our limited understanding of the interplay between the molecular structure, molecular packing, charge transport, and luminescence of organic semiconductors hampers the progress in the field. In this work, this interplay was theoretically and experimentally studied on a series of thiophene–phenylene co-oligomers, namely 5,5'-diphenyl-2,2'-bithiophene (PTTP) with seven different terminal substituents (bare, fluorine, methyl, trifluoromethyl, trimethylsilyl, tert-butyl, and methoxy), in crystals and field-effect devices. We revealed how the terminal substitution tunes the molecular packing, charge transport, and luminescence properties in the crystals. We found that the differences in the resolved crystal structures are mainly related to the inclination angle of PTTP molecules in the molecular layers, which is perfectly correlated with the van der Waals volume of the terminal groups and impacts the intermolecular interactions and molecular orbital overlap. We studied how charge transport depends on the inclination angle and found that PTTP with trimethylsilyl terminal groups has an optimal inclination supporting bipolar charge transport as demonstrated in organic-light emitting transistors (Fig.1). Moreover, this optimal inclination provides relatively weak dipole-dipole interactions corresponding to J-aggregation and results in the most resilience of crystal luminescence to molecular self-dopants efficiently capturing the excitation energy in the crystals with less inclined molecules forming H-aggregates. Finally, organic phototransistors based on the studied PTTP oligomers were demonstrated. We anticipate that our strategy and the revealed structure-properties relationships would greatly benefit the rational design of efficient organic optoelectronic materials.

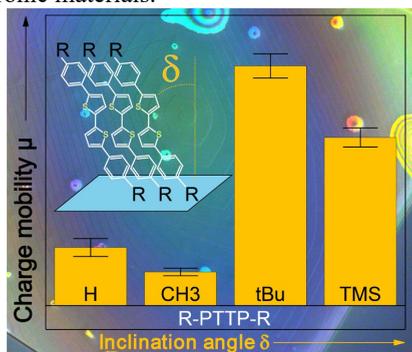


Fig. 1. Comparison of experimental and calculated (orientationally averaged) hole mobilities in the R–PTTP–R crystals.

*This work was supported by RSF (project № 22-79-10122).*

## Thiophene-Phenylene Co-Oligomers for Organic Field-Effect Phototransistors

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Organic electronics is a promising, rapidly developing field that has proven itself in the creation of such efficient devices as organic light-emitting diodes, organic transistors, organic solar cells and photodiodes. Also of interest are other promising devices based on organic materials, in particular, phototransistors studied in this work, which combine the properties of field-effect transistors and photodiodes.<sup>1,2</sup>

In this work research organic field-effect phototransistors based on thiophene-phenylene (P stands for phenylene, and T stands for thiophene) and annulated BTBT cores oligomers TMS-P4TP-TMS, TMS-PTTP-TMS, tBu-PTTP-tBu, BTBT-Ph, BTBT-Ph-F1. The maximum photocurrent values for phototransistors under uniform illumination of the channel with monochromatic optical radiation with an intensity of the order of 1 mW/cm<sup>2</sup> amounted to 0.20  $\mu$ A for the fluorinated annulated oligomer BTBT-Ph-F1. The maximum sensitivity values R were 0.7, 2.8, 0.7, 3.4 and 12.8 A/W for phototransistors based on TMS-P4TP-TMS, TMS-P2TP-TMS, tBu-PTTP-tBu, BTBT-Ph and BTBT-Ph-F1, respectively (Fig. 1b). External quantum efficiency (EQE) spectra were obtained for these phototransistors (Fig. 1a). The maximum value of the EQE was 41.8% for phototransistors based on BTBT-Ph-F1. For transistors based on the BTBT-Ph-F5 substance, the photocurrent was at the noise level (i.e., no photocurrent was detected).

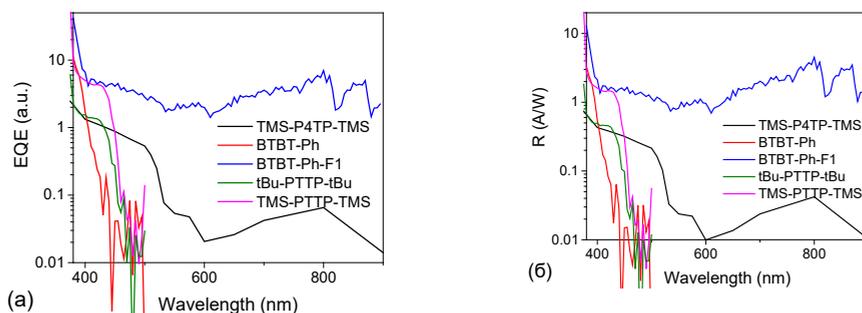


Fig. 1. Spectra of external quantum efficiency EQE (a) and sensitivity R of phototransistors based on polycrystalline layers of thiophene-containing and annulated oligomers TMS-P4TP-TMS tBu-PTTP-tBu, BTBT-Ph, BTBT-Ph-F1.

*This work was supported by RSF (project № 22-79-10122)*

<sup>1</sup> Baeg K., et al., *Adv. Mater.* 2013, **25**, 4267.

<sup>2</sup> Trukhanov V., et al., *Molecules*, 2024, **29**, 2533.

## Influence of Charge Carrier Mobility on the Form of Charge Carrier Recombination Rate Spatial Distribution in Organic Light Emitting Diodes

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One of the main problems in modern organic light-emitting diodes (OLEDs), especially in blue ones, is their insufficient lifetime in the operating conditions. One of the key reasons of OLEDs degradation is associated with the degradation of the organic emissive layers and their interfaces mainly within the electron-hole recombination zone, where the exciton density is high.<sup>1</sup> As a result, the energy density is high as well, which can result in a high probability of degradation.<sup>2</sup> The spatial profile of the recombination rate within the recombination zone is determined by mobilities of charge carriers, relative permittivity, as well as the misalignment of the HOMO and LUMO levels of the two materials at the interface of adjacent layers. In this work, using numerical modeling with the use of the drift-diffusion model, the dependence of the spatial distribution of the recombination rate of charge carriers on their mobilities has been revealed (Figure 1).

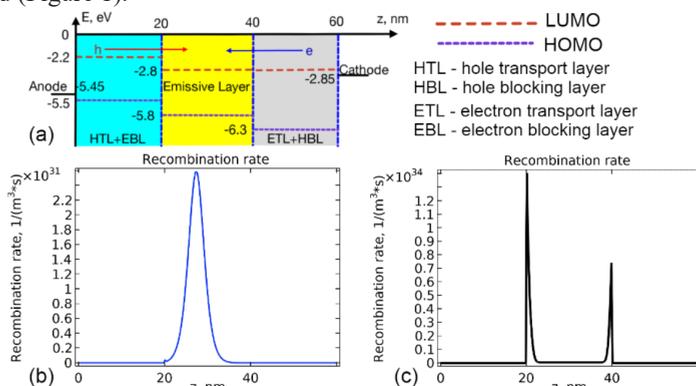


Fig. 1. OLED energy diagram (a), spatial distribution of the recombination rate of charge carriers ( $\text{m}^{-3}\cdot\text{s}^{-1}$ ) at an anode voltage of  $V_p = 9.5$  V for the same electron and hole mobilities equal to  $10^{-5}$   $\text{cm}^2/\text{V}\cdot\text{s}$  (b) and  $10^{-2}$   $\text{cm}^2/\text{V}\cdot\text{s}$  (c) in the emissive layer and  $10^{-2}$   $\text{cm}^2/\text{V}\cdot\text{s}$  in charge transport layers.

Figure 1c shows, that at high charge carrier mobility in the active layer ( $\sim 10^{-2}$   $\text{cm}^2/\text{V}\cdot\text{s}$ ), charge recombination regions are localized near the interfaces of the emissive layer with charge transport layers. At the lower charge mobilities in the active layer ( $\sim 10^{-5}$   $\text{cm}^2/\text{V}\cdot\text{s}$ ), a bell-shaped spatial dependence of the recombination rate is observed (Figure 1b). Consequently, the recombination area is distributed over the entire emission layer, and this should be beneficial for a long OLED lifetime. Unexpectedly, the high charge mobilities in the active layer could be a factor shortening the OLED lifetime. These findings can stimulate further development of more stable OLEDs.

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

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## Novel Annulated Organic p-Type Semiconductor: Synthesis and Properties

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The development of novel p-type organic semiconductor materials with the advantages of low-cost, designability of structure and flexibility<sup>1</sup> represents a significant challenge for the creation of highly efficient organic electronic devices. One of the most promising semiconducting materials in this field is rubrene (5,6,11,12-tetraphenyltetracene), which exhibits high charge carrier mobility of  $20 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$  at room temperature.<sup>2</sup> However, its practical use is severely limited by its instability to oxidation at room conditions.<sup>3</sup> This problem underlines the interest in structural design of this material providing its chemical derivatives or analogues with improved oxidative stability and enhanced device performance.

Here we report on a novel rubrene derivative with two methoxy-groups in para-position of side phenyl groups of rubrene backbone. The synthetic route was developed and optimized. All precursors and the target compounds were characterized by <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy and gel-permeation chromatography in an individual state. Optical and electrochemical properties, thermal and thermooxidative stability and phase behaviour of material were studied. Additionally, high stability of designed material towards photo-oxidation at room conditions in tetrahydrofuran solution was shown.

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

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<sup>1</sup> Zhang X. et al. *Adv.Mater.* 2018, **30**(44), 1801048.

<sup>2</sup> Podzorov V. et al. *Phys.Rev.Lett.* 2004, **93**(8), 086602.

<sup>3</sup> Ly J.T. et al. *J.Mater.Chem.C* 2018, **6**(14), 3757-3761.

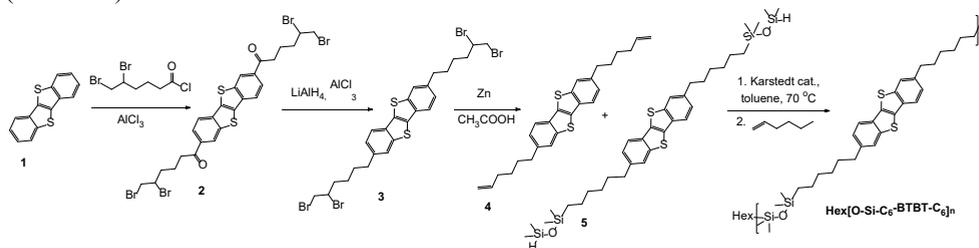
## Synthesis Strategy of a Novel Organosilicon Polymer with Dihexyl-Substituted [1]BenzoThieno[3,2-B][1]BenzoThiophene Fragments in the Main Chain

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Development, synthesis and investigation of properties of new organic semiconductive materials are one of the fast-moving topics in science. Such materials can be used as active layers in organic field-effect transistor (OFETs),<sup>1,2</sup> which in turn are applied in highly sensitive sensor devices.<sup>3</sup> The integration of functional fragments into a polymer chain makes it possible to produce materials with specified optoelectronic characteristics while maintaining high stability of the devices under normal environmental conditions. Combination of alkyl derivatives of [1]benzothieno[3,2-*b*][1]-benzothiophene (BTBT) with different polymers is known to lead to an increase in hole mobility in the semiconductor films and greater stability of the devices as compared to the initial low-molecular organic semiconductors.<sup>4</sup> Monolayer OFETs based on dialkyl-substituted BTBT siloxane dimer demonstrated high hole mobility and high air stability.<sup>5</sup> This work is devoted to the synthesis and characterization of a novel organosilicon polymer containing dihexyl-substituted BTBT fragments in the main chain (Scheme 1).



Scheme 1. Synthesis of the polymer **Hex[O-Si-C<sub>6</sub>-BTBT-C<sub>6</sub>]<sub>n</sub>**

The strategy for the synthesis of the target carbosilane-siloxane polymer **Hex[O-Si-C<sub>6</sub>-BTBT-C<sub>6</sub>]<sub>n</sub>** was based on the hydrosilylation reaction in the presence of Karstedt's catalyst. The synthesis of reaction monomer **4** was carried out with acylation according to the Friedel-Crafts method, followed by reduction of the keto group. At the final stage, a bromine deprotection reaction was carried out to form terminal double bonds. The preparation of monomer **5** was carried out with hydrosilylation reaction in the presence of Karstedt's catalyst.<sup>6</sup> This approach to the synthesis of organosilicon polymers with BTBT fragments in the main chain opens up broad prospects for obtaining new functional polymer materials for OFETs. Using polymeric materials gives the opportunity to apply modern technologies for application of the active layer in OFETs, for example, inkjet printing, due to the higher viscosity of such compound.

<sup>1</sup> Can A., Facchetti A., Usta H. *J. Mater. Chem. C* 2022, **10**, 8496–8535.

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<sup>3</sup> Wang Y., Zhang J., Zhang S., et al. *Polym. Int.* 2021, **70**, 414–425.

<sup>4</sup> Paterson A.F., Lin Y.-H., Mottram A.D. et al. *Adv. Electron. Mater.* 2018, **4**, 1700464.

<sup>5</sup> Trul A.A., Sizov A.S., Chekusova V.P. et al. *J. Mater. Chem. C* 2018, **6**, 9649–9659.

<sup>6</sup> Borshchev O.V., Sizov A.S., Agina E.V. et al. *Chem. Commun.* 2017, **53**, 885–888.

## Nanoparticles Based on Organic Conjugated Donor-Acceptor Molecules for Cancer Phototherapy

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Donor-acceptor (D-A) organic compounds are of significant importance in the field of modern organic electronics<sup>1</sup> and photonics<sup>2</sup>, due to the high mobility of charge carriers, photo- and hole conductivity, and efficient absorption in a range of spectral regions. These materials are employed extensively in the development of organic transistors, light-emitting diodes, solar cells and sensors. One of the principal advantages of D-A compounds is their capacity for structural modification, which enables the customisation of their optical and electronic properties in accordance with the specific requirements of the intended application. The use of D-A compounds in biomedicine is a recent and promising area of interest. Their low toxicity, high biocompatibility and tunable absorption, including in the near-infrared range, offer significant potential for the development of new materials for the diagnosis and treatment of diseases such as cancer.<sup>3</sup>

In this study, a series of D-A molecules based on triphenylamine (TPA) were synthesised. The high purity and given structure of the compounds were proved by a complex of modern physicochemical methods of analysis. An investigation into the relationship between the molecular structure and properties of these compounds will facilitate an enhanced efficacy in phototherapy and an improved specificity of their effects on cancer cells. This study examined the impact of the structural characteristics on the optical and electrochemical properties, phase behaviour and thermostability of the synthesised compounds. Then, aqueous dispersions of nanoparticles were prepared both based on the synthesized molecules and in combination with amphiphilic polymer matrices. The impact of encapsulation into the polymer on the size, stability and cytotoxicity of the nanoparticles was investigated. In some cases, the encapsulation of molecules into amphiphilic polymers resulted in an improvement in photodynamic properties, as evidenced by a change in the values of the half-maximal inhibitory concentration (IC<sub>50</sub>) and the phototoxic index (PI). The obtained systems have been demonstrated to possess a promising set of properties for photodynamic therapy, including efficient light absorption, photothermal conversion and heating, and high toxicity towards cancer cells. A confocal laser scanning microscope was employed to obtain fluorescence images, which demonstrated the generation of reactive oxygen species in cells using dichlorodihydro-fluorescein diacetate (DCFDA).

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

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<sup>3</sup> Lu B., Huang Y., Zhang Z., Quan H., Yao Y. 2022, **6** (20), 2968-2993.

**Biorecognition of Monoclonal Antibodies by EGOFET Based on Oligosaccharides**

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The problem of aspergillosis is aggravated by the increasing resistance of pathogens to antifungal drugs, as well as the appearance of multi-resistant strains. Early and accurate diagnosis of invasive aspergillosis is a serious problem because there is a wide range of non-specific clinical symptoms. One of the promising diagnostic methods is the development of biosensors.

Electrolyte-gated organic field-effect transistors (EGOFET) are a promising platform for ultra-sensitive, fast and reliable detection of biological molecules. The ability of label-free response using a simple electronic reading circuit is one of the main advantages of such devices compared to other identification technologies. With the help of EGOFET-biosensors, very low concentrations of analytes can be detected, which may correspond to diseases in the early stages.

*Aspergillus* cell wall components, such as oligosaccharides and glycoproteins, can be the basis of various biosensor platforms for detecting infection by *Aspergillus* species. Oligosaccharides can be integrated into the EGOFET due to a biotin-streptavidin platform located on the surface of the organic semiconductor layer of the device. And potential targets for analysis may be monoclonal antibodies that exhibit a specific interaction with oligosaccharides. Nowadays, the standard for determining mold fungi is a test based on *Limulus amoebocyte lysate* (LAL), but this method has a serious disadvantage – a large number of false positive results.

This work is aimed at studying the response of the bioreceptor layer in the EGOFET-biosensor containing biotinylated oligosaccharides related to galactomannan,  $\beta$ -(1 $\rightarrow$ 3)-D-glucan,  $\beta$ -(1 $\rightarrow$ 6)-D-glucan, which are part of the cell wall of the fungus *Aspergillus*, to monoclonal antibodies 7B8, 5H5, 1D2, specific to oligosaccharides, respectively, as a platform for rapid diagnosis of fungal disease. A specific response of the EGOFET-biosensor to oligosaccharides was demonstrated, as well as various control experiments were conducted. Based on the data of electrical characteristics and fluorescence microscopy, the selectivity of the device is shown. The concentrations of monoclonal antibodies detected using a biosensor are comparable to the results obtained by enzyme immunoassay based on antibodies and can compete with other test with advantage of rapidness of EGOFET sensors response.

*This work was carried out with the support of the Russian Foundation for Basic Research № FFSM-2022-0001*

## Circular Dielectric Elastomer Actuators Based on PDMS/MQ Composites

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Research in polymer chemistry has recently focused on developing new soft materials for soft robotics.<sup>1-3</sup> One highly promising class of soft transducers is dielectric elastomer actuators (DEAs). The advantages of DEAs include fast response, high energy density, and finetuneable actuation. Among the materials for DEA, silicone elastomers with high elongation are of most interest. High elongation provides long-term stability of the device and allows large deformations. Previously, it was clearly demonstrated that the efficiency of DEA depends on the ratio of the dielectric constant to the Young's modulus of the elastomer material.

This work presents the results of creation circular dielectric elastomer actuators composites based on polydimethylsiloxanes (PDMS) with different molecular weight and MQ-copolymers. (Fig.1) As a comparison, a similar actuator based on commercially available Elastosil 2030 silicone was obtained.

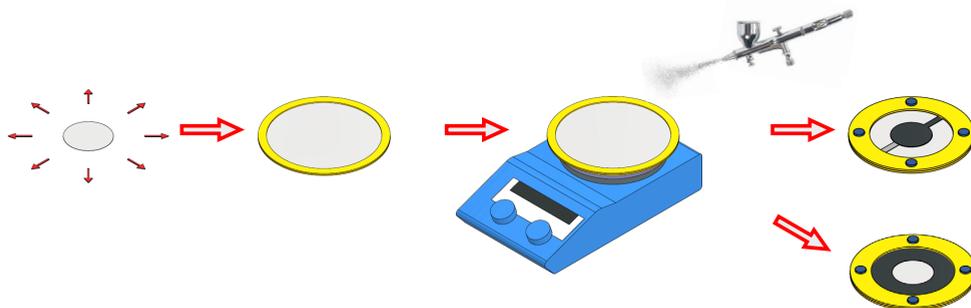


Figure 1. General scheme of creation cDEAs

It is found that despite the low dielectric constant, these composites demonstrate the best values of the parameter  $\epsilon_r/Y$  in comparison with other unmodified silicone materials, including commercially available ones, which, together with the wide possibilities of modification of PDMS/MQ composites, determines the prospects of their further use as a basis for the creation of DEA with low value of the actuation voltage.

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

<sup>1</sup> Bezsudnov, I. V. E., Khmel'nitskaia, A. G., Kalinina, A. A., Ponomarenko, S. A. *Uspehi himii*. 2023, **92**(2), 1-44.

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## Polyvinylidene Fluoride Grafted with Polyethyl Methacrylate Chains for Pressure Sensors

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Recently, a series of copolymers based on polyvinylidene fluoride with grafted polyethyl methacrylate (PEMA) chains were obtained by photoinduced reversible-deactivation radical polymerization (RDRP), and the effect of PEMA chains on their properties was investigated<sup>1</sup>. In particular, the study of thermal properties showed that an increase in the content of grafted chains in the copolymers leads to a decrease in the degree of crystallinity and improves film-forming properties, while it is accompanied by a decrease in the polymer degradation temperature. The grafted polymers obtained have good film-forming properties, therefore, studies were conducted and patterns were identified for the films of binary and ternary copolymers with different contents of grafted polyethyl methacrylate chains.

The possibility of using copolymers with PEMA as capacitive pressure sensors, for which the sensitivity and operating range varies with the change in the content of grafted PEMA chains, was investigated. Binary copolymers turned out to be more promising material for the pressure sensors, since they show high response reproducibility and low hysteresis (Fig. 1).

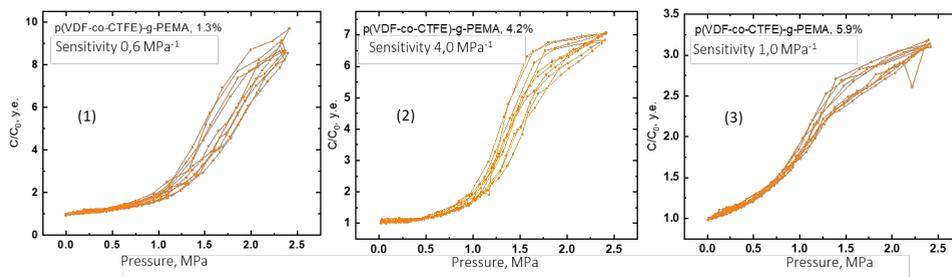


Fig. 1. Dependence of the relative capacitance on the applied pressure for the obtained p(VDF-co-CTFE)-g-PEMA films with a PEMA content of (1) 1.3%, (2) 4.2% and (3) 5.9%.

In addition, the copolymer films were filled with different amounts of barium titanate nanoparticles in order to track the change in permittivity and dielectric losses as compared to initial non-grafted polymers. The best result was shown by filled films based on the grafted copolymers with a small amount of PEMA chains compared to the initial non-grafted polymers.

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

<sup>1</sup> E.A. Klemyuk, A.I. Kosyakova, A.I. Buzin, V.G. Shevchenko, Yu.N. Luponosov, S.A. Ponomarenko. *Polym. Sci. Ser. C*, 2022, **64**, 200-210.

## Gentle Substrate Cooling in Vacuum Deposition of Small-Molecules Semiconductors

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Highly stable compounds with extended  $\pi$ -systems, macroheterocycles in particular, are in demand in organic electronic devices fabricated by thermal vacuum evaporation. They can serve as classical small-molecule semiconductors that absorb or emit light, or as buffer layers in complex multilayer hybrid devices, such as those based on perovskites. Flat or cone-shaped molecules of porphyrins and phthalocyanines usually form ordered films with different molecular packing or orientation of molecules relative to the deposition surface. The most popular approach to modifying the packing motif in such films is thermal annealing, either *in-* or *ex-situ*. This usually increases the crystallinity and surface roughness of the deposited films. In some applications, highly ordered layers are desirable, *e.g.* in thin-film field-effect transistors, where charge transport occurs within a 2D molecular network formed on the gate insulator. However, in photovoltaic cells, polycrystalline films are often not the target<sup>1</sup>, because they can undergo further (spontaneous or heat/light-induced) crystallization, resulting in output drift.

Recently, we developed a system for depositing thin molecular films with the substrate temperatures reduced to 258 K, in high vacuum chamber ( $\sim 10^{-6}$  Torr). The core of this system is a cascade of Peltier elements built into the substrate holder. In contrast to growth on substrates cooled to the liquid nitrogen temperatures<sup>2</sup>, the mild cooling does not stimulate intensive absorption of contaminants onto the surface of the growing film<sup>3</sup>. In this work, metal complexes of etioporphyrin M-EtioP (M=Ni, VO, InCl) were used; the films obtained at room and elevated temperatures were studied previously in our research<sup>4</sup>. It was found that vacuum deposition onto substrates cooled to 258 K leads to the formation of amorphous films without a typical fine-grained structure, while films grown at room temperature were highly textured. The morphological features of M-EtioP films are discussed in relation to their optical and charge-transporting properties. The examples of the use of “cold” molecular films in archetypal optoelectronic devices are considered.

*This work was supported by RSF (№20-13-00285-P).*

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<sup>3</sup> Forrest S.R. *Chem. Rev.* 1997, **97**, 1973-1896

<sup>4</sup> Pakhomov G.L. et al. *ChemistrySelect* 2023, **8**(45), e202303271

## The Specificity of the Sensitivity of Organic Field-Effect Transistors with Various Interface Dielectrics

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In the pursuit of developing affordable portable gas analysers, an emerging and promising strategy entails the use of thin-film organic field-effect transistors (OFETs) with semiconductor layers responsive to various atmospheric compounds<sup>1</sup>. Although the electrical and sensory properties of OFETs have been widely explored, the impact of the interfacial dielectric material on these properties remains a critical area of investigation.

In this work, the role of interface dielectric materials in sensory properties (to NO<sub>2</sub>, SO<sub>2</sub>, and NH<sub>3</sub>) of BTBT-based OFETs was investigated. Widely used polymer and non-polymer interface layers such as PMMA (Polymethylmethacrylate), PS (Polystyrene), CYTOP (Cyclized Transparent fluorinated Optical Polymer), ODMS (Octadecyldimethylchlorosiloxane) were used in this study. The OFETs without any interface layer were also investigated as reference devices. During study, the sensory properties of OFETs were analysed in conjunction with their electrical properties and layer morphology.

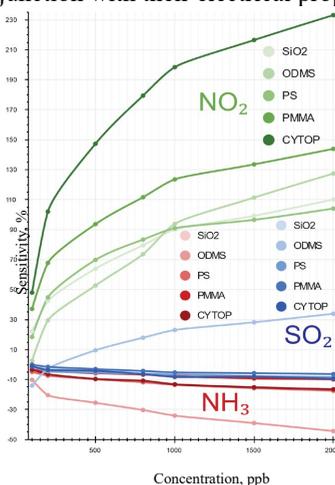


Fig. 1. The graph shows the dependence of the sensitivity of transistors on different interface layer materials and different concentrations of three tested gases.

The results (Fig. 1) demonstrate a significant dependence of sensory characteristics on selected dielectric materials. For instance, sensors with CYTOP interface layers exhibited a pronounced positive response to NO<sub>2</sub>, while demonstrating slight negative responses when exposed to SO<sub>2</sub> and NH<sub>3</sub>. In contrast, devices with ODMS showed significant responses varying in sign in experiments involving SO<sub>2</sub> and NH<sub>3</sub>. These findings underscore the importance of selecting an appropriate dielectric layer, as it significantly influences interactions with toxic gases, thereby affecting the device's suitability for practical applications.

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

<sup>1</sup> A. A. Trul et al., *J Mater Chem C*, 2018, **6**, 9649-9659.

### Ternary Composite of Polymer, Fullerene and Fluorinated Multi-Walled Carbon Nanotubes as the Active Layer of Organic Solar Cells

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Fluorinated multi-walled carbon nanotubes (F-MWCNTs) are utilized as the third component in the active layer of organic solar cells. A method for producing F-MWCNTs has been established, and adding these nanotubes in amounts ranging from 0.25% to 2% by weight to the active layer improves device characteristics such as fill factor (FF), short-circuit current density (J<sub>sc</sub>), and power conversion efficiency (PCE).

Incorporating roughly 1% by weight of these nanotubes into the PCDTBT/PC60BM polymer/fullerene active layer results in a significant enhancement of key photovoltaic parameters, including stability. This effect is likely due to the optimization of the donor/acceptor composite morphology and the structural reinforcement provided by the F-MWCNTs. Evidence supporting this theory is found in the substantial impact of the F-MWCNT additive on the kinetics of the decay of the EPR signal of light-induced charges within the PCDTBT/PC60BM composite.

Overall, this addition results in an approximate 20% increase in PCE. The enhancement in device performance is thought to stem from modifications to the active layer's morphology due to the introduction of MWCNTs. The reduction of energetic disorder for charge transfer in the PCDTBT/PC60BM composite upon adding F-MWCNTs provides indirect evidence of changes in the nanomorphology of this composite. Additionally, the inclusion of F-MWCNTs enhances cell efficiency over extended periods, exceeding 1200 hours, likely by stabilizing the thermodynamically unstable morphology of the bulk heterojunction active layer and reinforcing it.

*This work was supported by RFBR (project № 23-73-00072).*

**I-Motif Aptamer for Biosensing by Electrolyte-Gated Organic Field-Effect Transistors**

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Electrolyte-gated organic field-effect transistors (EGOFET) are widely used as a platform for biosensors, providing low analyte detection limits and high specificity. Antibodies, enzymes, proteins, and aptamers are used as recognition elements for biosensors based on EGOFET. Compared to antibodies and enzymes, aptamers are resistant to heat, pH changes and chemically aggressive conditions. Therefore, aptamers are more effective substances for practical use. The use of aptamers opens up a method for sensitive, selective and affordable detection of biomolecules. Furthermore, due to their unique structure, aptamers can be used to detect multiple analytes under different conditions. This property of aptamers was investigated in this work to determine the possibility of controlling the properties of biosensors based on EGOFET using an aptamer with i-motif structure.

The previously described approach to manufacturing a biosensor with an active semiconductor layer based on C8-BTBT-C8 in a mixture with polystyrene and a bioreceptor layer based on the siloxane dimer BTBT and the biotin derivative BTBT-biotin was used as the EGOFET platform<sup>1</sup>. This platform provides biotin-streptavidin interaction on the surface of the semiconductor layer of the EGOFET. The streptavidin layer was functionalized with the recognition element aptamer BV42, which has an i-motif structure and binds influenza A virus virions at pH 6. The absence of shift in threshold voltage and transfer conductivity of biosensors based on EGOFET at pH 6 and pH 8 was demonstrated. BV42 is able to bind silver cations, forming an organometallic complex cytosine-Ag<sup>+</sup>-cytosine, causing a shift in the saturated mode transfer conductivity ( $g_m$ ) of the EGOFET-based biosensor at pH 8. Aptamer BV42 is pH-dependent in the pH range from 6 to 8, which can be used to determine the pH of the environment in the range significant for biological measurements. The sensitivity of the i-motif aptamer based sensor lies in the same range as for the aptamer RHA0385, published earlier<sup>1</sup>.

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

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<sup>1</sup> Poimanova E.Yu, Shaposhnik P.A, Anisimov D.S, et al. *ACS Appl Mater Interfaces*. 2022, **14**(14), 16462-16476.

## Crown Ether-Based Electrolyte-Gated Organic Field-Effect Transistor for Detection of Alkali Metals

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The creation of a sensor capable of quickly and selectively reacting to alkali metal ions in biological fluids is a promising task for the development of a simple and mobile multi-sensor device capable of monitoring a person's condition outside a medical institution. This work is a development of an earlier study<sup>1</sup> and is aimed at developing a new semiconductor compound based on crown ether and benzothiene[3,2-*b*]benzothiophene (BTBT), as well as creating a full-fledged electrolyte-gated organic field-effect transistor (EGOFET) device using the resulting compound as a component of the receptor layer for recognizing potassium ions in a solution of real biological fluids. The proposed approach to creating a receptor layer of the device is based on the Langmuir-Schaeffer method and provides the possibility of creating a universal platform for further recognition of alkali metal ions through the use of structures containing crown ether groups binding to a previously developed universal support layer<sup>2</sup> without significantly deteriorating the electrical properties of the EGOFET device.

In the course of this work, the synthesis of a compound containing a conjugated fragment of BTBT and 4,13-diaza-18-crown-6 ether, acting as a receptor anchor for capturing ions from the analyte solution, was carried out (Fig. 1).

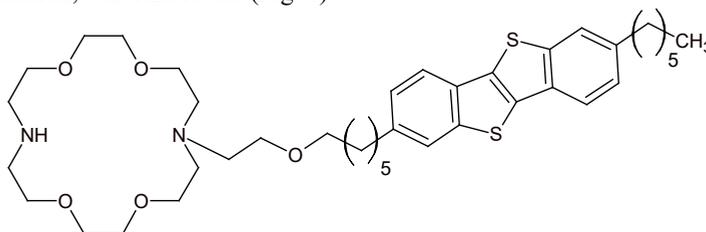


Figure 1. Structural formula of the synthesized compound.

A technique has been developed for manufacturing an EGOFET device with a receptor layer that allows selectively binding potassium ions in solutions with high ionic strength. Several devices have been manufactured that show stable operation in deionized water. The electrical characteristics of the obtained devices were measured, and the surface was analyzed in order to assess the quality of the obtained monolayer films. Currently, further work is underway to find optimal parameters for measuring the response to potassium ions, measuring the selectivity and sensitivity of the devices obtained. It is planned to create a full-fledged device capable of determining the concentration of potassium ions in solution in real time.

*This work was supported by Russian Science Foundation (grant 19-73-30028).*

<sup>1</sup> B.S. Kuleshov, E. Y. Poymanova, M. S. Skorotetsky, O.B. Borshchev, G.V. Cherkaev, E. V. Agina, S. A. Ponomarenko. *Russian Chemical Bulletin - In print.*

<sup>2</sup> Trul A.A., Sizov A.S., Chekusova V.P., et al. *J Mater Chem C Mater.* 2018; **6**(36):9649-9659.

## Inkjet Printed Organic Semiconductor Devices Based on C8-BTBT Materials

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Organic semiconductors combine a range of advantages such as flexibility, low trap density and high mobility of charge carriers. These features provide great potential for their application in organic field effect transistors (OFET). In this work we demonstrate a simple and effective method of 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene (C8-BTBT)<sup>1</sup> film fabrication by inkjet printing (IP). IP is characterized by low material consumption, non-contact deposition and control of the printing ink location with a given pattern<sup>2</sup>.

The grain size and crystal orientation of organic thin films obtained by solution methods directly depend on manufacturing conditions, such as solvent evaporation rate and liquid surface tension. The addition of polystyrene (PS) allows to optimize the solution viscosity for printing methods and it also effect on the formation of a highly homogeneous crystalline semiconductor thin films by reducing of rate crystallization C8-BTBT<sup>3,4</sup>. Therefore, the purpose of this work was to study the approaches to optimizing of the ink solution composition based on C8-BTBT:PS to inkjet printing. Working devices with different C8-BTBT:PS ratios were prepared – 1:0, 10:1, 4:1 and 2:1, as well as with different concentrations of PS in solution – 0.5; 1.25; 3.7 and 7.5 g/L. The films obtained without the addition of PS did not cover the entire surface of a given pattern, that is, they had poor adhesion to the substrate (Fig.1). And with an increase in the concentration of PS in the solution, the threshold voltage of the OFETs increased. The effect of the composition of the C8-BTBT:PS mixture and the concentration characteristics of the solution on the performance of OFETs will be reported.

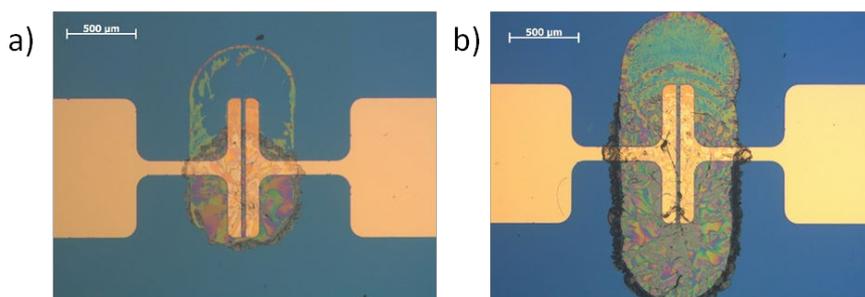


Fig. 1. Optical micrographs of inkjet-printed films of C8-BTBT (a) and C8-BTBT:PS (b).

*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 with MIPT in the framework of grant No. 075-15-2024-560).*

<sup>1</sup> Ebata H. et al. *J. Am. Chem. Soc.*, 2007, **129**, 15732.

<sup>2</sup> Titova Ya.O. et al. *Russ. Chem. Bull.*, 2023, **72**, 1130–1138.

<sup>3</sup> Xie P. et al. *Sci. Bull.* 2020, **65** (10), 791-795.

<sup>4</sup> Shaposhnik P.A. et al. *Dokl. Phys. Chem.*, 2021, **496**, 20–24.

## Conductivity of Filled Polymers Modelled by the Cooperative Systems Approach

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In the theoretical study of the behavior of carbon-filled silicone polymers, a model of the behavior of the conductivity of such materials was proposed using the framework of cooperative agent systems (CAE). In the model, the agents (filler clusters) are born, grow and then collapse but touching each other the agent's clusters get the extended lifespan - bonus. The mechanical load applied to the composite leads to a change in its structure, i.e. the emergence, growth and disappearance of clusters of filler particles, the clusters that arise during compression can also collapse during the relaxation or over pressure of the composite.

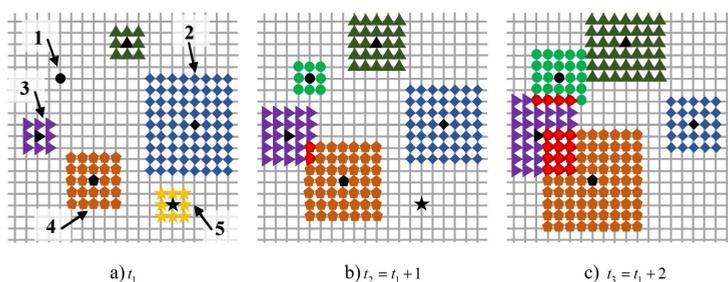


Fig. 1. CAE model on the 2D square regular lattice. Birth, development, and dying of agents, three consecutive time steps. Agent 1 is born at  $t_1$  and further develops on steps  $t_2$  and  $t_3$  (green), Agent 2 develops more than the initial lifespan  $T_0$  time steps, on further steps it will shrink and soon will die (blue), Agents 3 and 4 grow (brown and violet) and on the step  $t_2$  form the cluster (common nodes are in red) and their lifespan will be increased by  $T_b$ . Agent 1 on the step  $t_3$  joins the cluster of 3&4. After step  $t_3$ , Agents 3 and 4 have a bonus  $2T_b$ , and the Agent 1 – bonus  $T_b$ . Agent 5 (yellow) dies and disappears at the step  $t_3$ .

The affinity of the particles of the carbon filler, the possibility of their mechanical interlocking, etc. will restrain the process of destruction and promote the preservation and growth of filler agglomerates. Thus, the formation of large agglomerates and, then, an emergence of inclusions network leads to a sharp increase in the conductivity of the carbon composite, as a rule, this occurs similarly to the behavior of percolation systems near the percolation threshold. In the present model, threshold phenomena also arise and it is shown that the threshold depends on the degree of affinity of the filler particles, in terms of work on agent systems - a bonus. The emergence of an infinite cluster, including the appearance of conductivity of the composite, depends on the size of the bonus, the larger it is, the faster the infinite cluster arises. In the model system, a transition close to percolation also occurs, demonstrating behavior similar to composites under load.

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## A New Approach to the Production of Organosilicon Photo Conversion and Photo-Curable Films

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An important component in the development of new technologies for displays, LEDs, and solar cells is photoconversion coatings. Oligomer matrices and luminophores are used to create such coatings. In a previous study on this topic, the results using red-luminophore VDM-2T-BTD-2T-VDM<sup>1</sup> as the luminescent material and organosilicon thiol- and vinyl-containing oligomers as the matrix were presented.<sup>2</sup> However, this material did not exhibit the desired properties: resistance to environmental factors and a low quantum yield, which was caused by the aggregation of the phosphor molecules.<sup>3</sup>

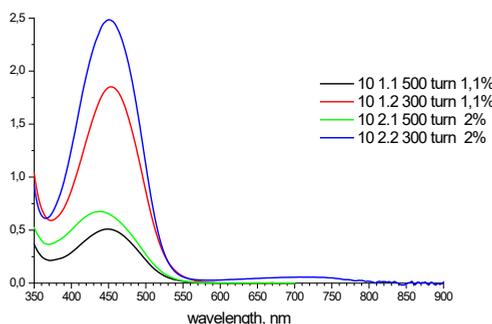


Fig. 1 – Absorption spectra.

In this work, we conducted the synthesis of a new oligomeric matrix and developed coatings based on it using a phosphor that contains fewer thiophene units in its structure. The new matrix includes oligosiloxane oligomers with phenyl ring content, which enhance the stability and hardness of the structure in the film. The introduction of phenyl rings into the structure promotes a sparser spatial crosslinking, which reduces the quenching of luminescence. The use of VDM-T-BTD-T-VDM enabled us to achieve a quantum yield of 50% in the film due to the absence of aggregation in the matrix. Moreover, the obtained films exhibited high values of optical density (see Fig. 1). Such an increase in the performance of the films opens new horizons for the study of photo conversion coatings.

*This work was supported by Ministry of Science and Higher Education (project FFSSM-2022-0004)*

<sup>1</sup> M. S. Skorotetcky, E. D. Krivtsova, O. V. Borshchev, N. M. Surin, E. A. Svidchenko, Y. V. Fedorov, S. A. Pisarev, and S. A. Ponomarenko. *Dyes and Pigments*, 2018, **155**(8), 284-291.

<sup>2</sup> M. N. Temnikov, Y. N. Kononevich, I. B. Meshkov, M. I. Buzin, V. G. Vasil'ev, G. G. Nikiforova, and A. M. Muzafarov., *Polymer*, 2018, **138**, 255-266.

<sup>3</sup> *D.K. Gaikov, O.V. Borschev, S.A. Ponomarenko* A new approach to the production of organosilicon fluorescent photo-curable films. *III All-Russian School Conference with international participation on Biocompatible Electronics and Robotics*, 37, (2024)

## Tuning of Physical and Chemical Properties of Dithienyl Derivatives of [1]BenzoThieno[3,2-B] [1]BenzoThiophene by Variation of the Position of Solubilizing Alkyl Groups

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Derivatives of [1]benzothieno[3,2-b][1]benzothiophene (BTBT) are one of the most popular types of compounds for use in basic elements of organic electronics – organic field effect transistors (OFETs) with high mobility. Excellent chemical and thermal stability of the BTBT fragment allows both variation of conjugated substituents and solubilizing groups or groups that contribute to the self-organization of semiconductor molecules in crystals. The high degree of planarity of molecular semiconductors and the ability to self-organize, along with high processability, allows the use of BTBT derivatives in elements with different configurations: high performance OFET, electrolyte gated OFET, organic light emitting transistors, phototransistors, etc<sup>1</sup>.

In addition to these peculiarities, it is possible to vary the position of solubilizing substituents in conjugated fragments. However, currently there are no publications covering the simultaneous study of the effect of the position of the aliphatic substituents on optoelectronic, thermal and electrophysical characteristics of BTBT derivatives.

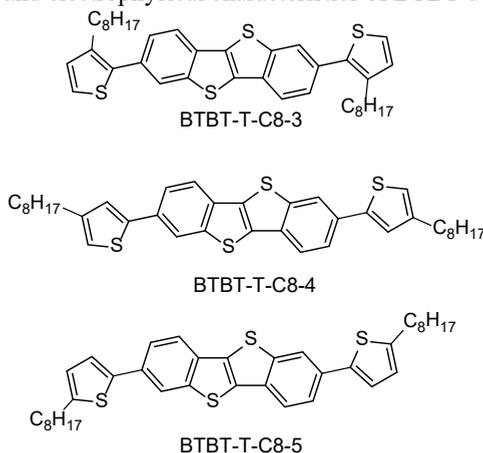


Fig. 1. Novel dithienyl derivatives of BTBT with different positions of alkyl substituents

Three novel dithienyl derivatives of BTBT derivatives with solubilizing groups in 3, 4 or 5 positions of thienyl rings were synthesized via Suzuki cross-coupling reactions and isolated in pure form (Fig.1). The effect of the position of the alkyl substituents on the optoelectronic, thermal and electrophysical properties of these derivatives of BTBT will be presented.

*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).*

<sup>1</sup> P. Xie, T. Liu, J. Sun, J. Yang. *Adv. Funct. Mater.* 2022, **32**, 2200843.

## Blue Organic Light-Emitting Diodes Based on New Multi-Resonance Fluorescence Materials

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Organic light-emitting diodes (OLEDs) are one of the most promising types of light emitting devices for display technologies due to their low operating voltage, fast response, high brightness as well as flexibility. Blue OLEDs have attracted particular attention from the scientific community because of their stability problems, so they require intensive research. The third generation OLEDs based on thermally activated delayed fluorescence (TADF) materials are the most efficient. In such devices the internal quantum yield of electroluminescence can reach 100%. The molecular structure of TADF-luminophores contains donor and acceptor fragments. The highest occupied molecular orbital (HOMO) is localized mainly on donor fragments, and the lowest unoccupied molecular orbital (LUMO) - mainly on acceptor fragments. As a result, the degree of overlap between HOMO and LUMO is relatively small, resulting in efficient delayed fluorescence. However, this TADF-luminophore structure is not without disadvantages such as low oscillator strength of the S<sub>1</sub>-S<sub>0</sub> transition and wide emission bandwidth, which is critical for display technologies due to reduced color purity. These disadvantages can be overcome by multi-resonance luminophores, in which the spatial separation of frontier molecular orbitals is realized on alternating donor and acceptor atoms, rather than on polyatomic donor and acceptor molecular fragments<sup>1</sup>. In such materials, the local electron-phonon interaction is suppressed, resulting in a narrow luminescence spectrum and high color purity. One of the promising variants of such structures for blue OLEDs are indolocarbazole and carbazolylene derivatives<sup>2,3</sup>. In this work, we fabricated and characterized blue OLEDs based on indolocarbazole (MR1) and carbazolylene (MR2) derivatives (Fig.1) with device structure: glass/ITO/PEDOT:PSS/BT-TBA/NaNaP-A(host):MR1 or MR2(dopant)/Bepq2/Ca/Al. Electroluminescence spectra, external quantum efficiency, brightness and other OLEDs parameters were measured and discussed.

a)



b)

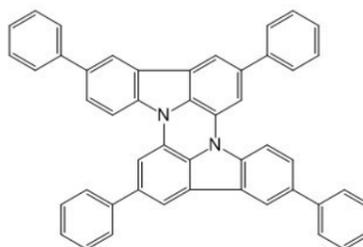


Fig. 1. Chemical structures of MR molecules: a) MR1, b) MR2.

*This work was financially supported by Ministry of Science and Higher Education of the Russian Federation, project № FF5M-2022-0004.*

<sup>1</sup> T. Hatakeyama, et al. *Advanced Materials*. 2016, **28**, 2777–2781.

<sup>2</sup> G. Meng, et al. *Chemical Science*. 2022, **13**, 5622–5630.

<sup>3</sup> C. Cheng, et al. *Chemical Engineering Journal*. 2023, **474**, 145691.

## Indolocarbazole- and Diindolophenazine-Based Fluorophore with High-Efficiency Blue Electroluminescence

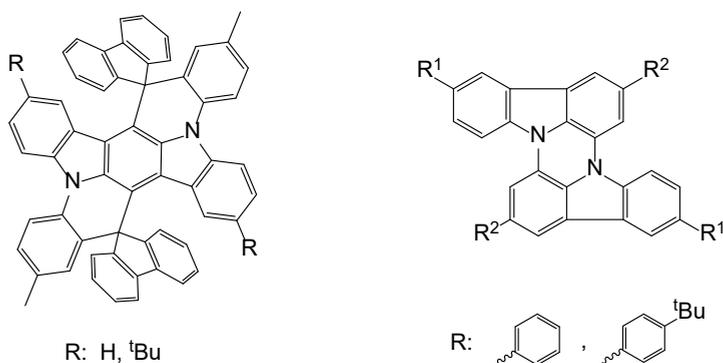
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The development of reliable blue OLEDs with high efficiency and stability is still an immediate task, since their characteristics largely lag behind the green and red ones.<sup>1</sup> Thus, significant efforts have been made to improve the performance of blue OLED displays. Recently, due to conceptual advances in molecular design, sky-blue OLED displays based on phosphorescence or thermally activated delayed fluorescence materials as emitters or sensitizers for fluorophores have been rapidly developing both in terms of efficiency and service life. In this work, we obtained both known<sup>1,2</sup> and new fluorophores based on indolocarbazole and diindolophenazine cores for blue OLEDs.



*This work was supported FFSM-2022-0004.*

<sup>1</sup> Meng, G., Zhang, D., Wei, J., Zhang, Y., Huang, T., Liu, Z., ... & Duan, L. *Chemical Science*, **13**(19), 5622-5630.

<sup>2</sup> Cheng, C., Zhu, Y., Tsuboi, T., Deng, C., Lou, W., Liu, T., ... & Zhang, Q. *Chemical Engineering Journal*, **474**, 145691.

## Tuning the Morphology of PM6/Y6 Active Layer of Organic Solar Cells Via Intermediate Ternary Donor/Acceptor/Volatile Additive Blend

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2-(2-Methylphenyl)benzo[b]thiophene (MPBT) was synthesized and applied as volatile additive to PM6/Y6 active layer of organic solar cells. Typically, volatile additives are removed from this composite by subsequent thermal annealing, which is accompanied by change of the molecular packing within donor and/or acceptor domains. Due to volatility of MPBT, annealing at 120 °C allows its complete removal from PM6/Y6 composite. However, its morphology is markedly altered by MPBT, as it is evidenced by optical spectroscopy and atomic force microscopy. For thin PM6/Y6 active layer (about 70 nm thickness) cast from chlorobenzene the optimal concentration of MPBT is 5 % wt:wt, relative to the solvent. Use of this additive leads to improvement of short circuit current  $J_{SC}$  and fill factor, and consequently, to power conversion efficiency (PCE) increase. External quantum efficiency (EQE) improves within the whole range of PM6/Y6 optical absorption (350 – 850 nm). For thick PM6/Y6 active layer (about 250 nm) cast from chloroform the optimal concentration of MPBT is only 0.5 % wt:wt, which leads to improvement of all photovoltaic parameters. Presumably, the origin of the photovoltaic performance improvement is optimization of the morphology of PM6/Y6 active layer during formation of the ternary composite PM6/Y6/MPBT upon spin-coating and removing of MPBT from this composite upon thermal annealing. Study of MPBT influence on Y6 shows significant change of optical absorption of Y6 films upon thermal annealing. Intensity changes in optical spectra upon annealing can be explained by delocalization of excitons in Y6 films annealed in presence of MPBT, similarly to the case of semicrystalline polymer P3HT. The exciton delocalization can be caused by closer packing of Y6 molecules in MPBT-processed films. In particular, optical, XRD and AFM data point to crystallization of Y6 during MPBT volatilization. SCLC electron mobility increases several times upon volatilization of MPBT from PM6/Y6 film, while hole mobility remains essentially unchanged. Overall, novel approach based on intermediate donor/acceptor/additive ternary blend gives additional degree of control active layer morphology in OPV devices.

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

## Catalyst-Free Synthesis of Carbazolyl-Containing Fluorophores as Perspective Functional Materials

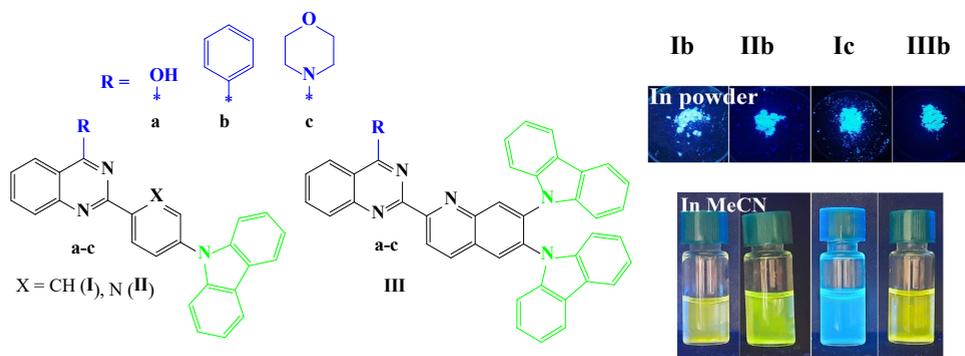
*T.N. Moshkina*<sup>1\*</sup>, *M.I. Valieva*<sup>1</sup>, *E.S. Starnovskaya*<sup>1</sup>, *E.V. Nosova*<sup>1</sup>

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Organic fluorophores containing  $\pi$ -deficient quinazoline core are under high interest as functional materials with semiconducting, emissive, sensory or detection properties across various applications. Carbazole derivatives due to high morphological and thermal stability, variety of synthetic approaches and modifications are widely used in molecular electronic materials, such as organic light-emitting diodes like blue, green, red, and white emitters or as dye sensitive solar cells.<sup>1,2,3</sup>

Carbazolyl-substituted quinazolines **I**, **II** and **III** were synthesized by treatment of fluoro-substituted 2-aryl(azinyl)quinazoline with sodium carbazole salt generated *in situ* from carbazole and NaH.



Comp	$\lambda_{\text{abs}}$ , nm ( $\epsilon$ , $10^4 \text{ M}^{-1}\text{cm}^{-1}$ )	$\lambda_{\text{em}}$ , nm	$\Delta\nu$ , $\text{cm}^{-1}$	QY, %
<b>Ib</b>	257 (4.73), 328 (1.83), 339 (1.79)	550	11317	26
<b>Ic</b>	329 (3.15), 338 (3.06)	464	8034	42
<b>IIa</b>	336 (1.57), 350 (1.58)	517	9229	27
<b>IIb</b>	255 (4.08), 336 (1.46)	524	10678	39

\*In MeCN

Obtained compounds demonstrated fluorescent properties in blue or yellow region and moderate quantum yield in MeCN. Moreover, all compounds were found to be emissive in solid state.

*This work was supported by Russian Science Foundation (project № 23-73-01147)*

<sup>1</sup> Bélières M., Sartor V., Fabre P.L., Poteau R., Bordeau G., Chouini-Lalanne N. *Dye Pigment*. 2018, **153**, 275–283.

<sup>2</sup> Sathiyar G., Sivakumar E.K.T., Ganesamoorthy R., Thangamuthu R., Sakthivel P. *Tetrahedron Lett*. 2016, **57**, 243–252.

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## Synthesis and Properties of New Non-Fullerene Acceptors for Organic Solar Cells

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Currently, organic photovoltaics, particularly organic solar cells (OSCs), are a subject of great interest to the global scientific community, as OSCs represent an environmentally friendly technology of renewable energy. The power conversion efficiency (PCE) of OSCs exceeds 19%<sup>1,2</sup> for devices based on fused ring non-fullerene electron acceptor materials (FREAs), which are complex polyaromatic compounds of the donor-acceptor type with a planar and rigid chemical structure. For less complex NFAs of non-fused ring structure (NFREAs) with bulk substituents in the structure that prevent conformational transitions of the molecule, the PCE achieves 17%<sup>3</sup>. Notwithstanding the aforementioned successes, the most significant challenge to the commercialization of OSCs based on FREAs is the labor-intensive and multistep nature of their synthesis, which renders these materials prohibitively expensive. The realization of NFREAs is still hindered by the unresolved issues of stability, complementarity of donor materials for them, and structure-property-performance relationship of the device. Moreover, the utilization of NFAs that absorb within the NIR range of 750 to 1200 nm can markedly extend the absorption spectrum of the active layer and augment the photon collection capacity of OSCs, thereby enhancing efficiency. Consequently, the pursuit of structures with the requisite physicochemical attributes to develop high-efficiency OSCs is crucial and pertinent.

This work presents the synthesis of new potential NFAs, which were developed and carried out. The chemical structure of the compounds were proved by <sup>1</sup>H NMR, <sup>13</sup>C NMR techniques and by MALDI mass spectrometry analysis. The compounds are characterized by a high thermal and photo stability, efficient sunlight absorption in the red and near-infrared spectral ranges, good solubility combined with a high degree of crystallinity and possess appropriate energy levels of HOMO and LUMO levels to be used for OSCs. The photovoltaic data of the novel NFAs in binary and ternary blends with commercially available donor material PM6 and acceptor material Y6 demonstrated PCE of more than 18% in prototype ternary OSCs, which is comparable to the record values in this field.

*The work was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation (Agreement No. 075-15-2024-532 dated 24.04.2024)*

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<sup>2</sup> Wan, J., Dyadishchev, I., Sun, R., et al. *J. Mater. Chem. A.* 2022, **10**, 17122-17131.

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## Synthesis and Structure-Property Relationship Study for New Push-Pull Fused Oligomers Based on Indole[3,2-B]Indole and BenzoThieno[3,2-B]BenzoThiophene

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Organic semiconductor materials are being developed and researched very actively, which opens up opportunities for the development of many modern fields of science and technology. Before the synthesis of new substances, it is extremely important to competently consider their structure, as it will depend not only on the conductive and electrochemical properties of future compounds, but also on their phase behavior, solubility, the ability to certain types of packing in the crystal, which affects the electrical characteristics and the possibility of creating devices based on them<sup>1</sup>. The structures represented by the combination of electron-donor (D) and electron-acceptor (A) parts (D-A) are very interesting, since the variation of different strength and nature of D and A units makes it possible to control in a wide range of molecular energy levels, achieving the desired properties in the resulting compounds<sup>2</sup>. Organic molecules consisting of condensed heteroaromatic links are of particular interest. The rigid structure of such compounds provides  $\pi$ -conjugation with good conductivity, high oxidation stability and dense molecular packing<sup>3</sup>.

A number of semiconducting oligomers of D-A structure have been obtained (Fig. 1.), which have donor heteroaromatic units in their basis: the well-known benzothieno[3,2-b]benzothiophene<sup>4</sup> and indole[3,2-b]indole; acceptor functional groups (keto- and dicyanovinyl); benzene and thiophene conjugated  $\pi$ -spacers as a connection between the D and A parts of the molecules.

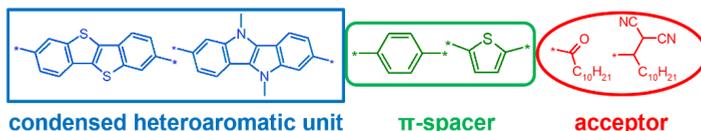


Fig. 1. Schematic structure of oligomers

Synthesis schemes of new oligomers and results of studies of electrochemical, optical and thermal properties, phase behavior of substances will be presented. Based on the obtained data, the interrelationships between the structure and properties of the obtained series of oligomers will be revealed and presented, namely, how the replacement of individual parts of the molecule affects the final properties. Prospects of application of the obtained materials in applications of organic and hybrid electronics will be evaluated.

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

<sup>1</sup> Bronstein H., Nielsen C.B., Schroeder B.C. *Nature Reviews Chemistry*. 2020, **4**, 66-77.

<sup>2</sup> Toshiki H., Takehiko M. *Phys. Chem. Chem. Phys.* 2022, **24**, 9770-9806.

<sup>3</sup> Zhang W., Liu Y., Yu G. *Advanced Materials*. 2014, **26**, 6898-6904.

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## Novel TADF-Polymers for 3<sup>th</sup> Generation OLED Materials

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The powered development of diverse wearable electronic devices requires to employing of high-performance organic light-emitting diodes (OLED) that are concerned with the obtaining of new materials<sup>1</sup>. There are three generations of OLED materials: fluorescent organic materials (1<sup>st</sup> generation), phosphorescent organometal complexes (2<sup>nd</sup> generation) and organic molecules with thermal active delayed fluorescence (TADF) feature (3<sup>th</sup> generation). It is known that newest compound class can achieve 100% internal quantum efficiency that is based on the possibility to enhance emitting from singlet state by reverse intersystem crossing and by tiny difference between singlet and triplet energy states.

Polymeric light-emitting diodes (PLED) are promising group of OLED devices that consist of polymers with electroluminescent ability enhanced by TADF. A number of PLED are synthesized and characterized<sup>2</sup>. Today we have results of literature study and polymers with non-conjugated chain and donor/acceptor pendant groups (Fig.1) based on it. This work presents the compiled literature data, early synthetic results and optical study of obtained polymers.

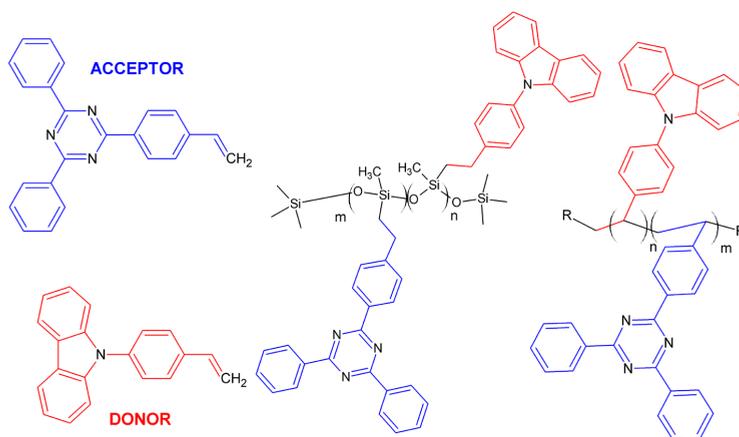


Fig. 1. Molecules used in the synthetic route.

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

<sup>1</sup>Endo A., Ogasawara M., Takahashi A., Yokoyama D., Kato Y., and Adachi C. *Adv. Mater. Weinheim* 2009, 21, 4802–4806.

Guo J. J., Li X. L., Nie H., Luo W. W., Gan S. F., Hu S. M., et al. *Adv. Funct. Mater* 2017, 27, 13.

<sup>2</sup>Yin X., He Y., Wang X., Wu Z., Pang E., Xu J and Wang J. *Front. Chem.* 2020 8:725.

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Yang Y. K., Wang S. M., Zhu Y. H., Wang Y. J., Zhan H. M., and Cheng Y. X. *Adv. Funct. Mater.* 2018a, 28:1706916.

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## Study Of Influence of Terminal Groups in 2,1,3-Benzothiadiazole-Based Thiophene-Phenylene Derivatives

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Recently, there has been a significant interest in donor-acceptor systems for organic electronic applications. Researchers are actively working to enhance the properties of molecules by modifying individual components.<sup>1</sup> 2,1,3-Benzothiadiazole (BTD) is commonly utilized as an acceptor unit owing to its impressive optoelectronic characteristics and its ability to form efficient luminophores when paired with donor units.<sup>2</sup>

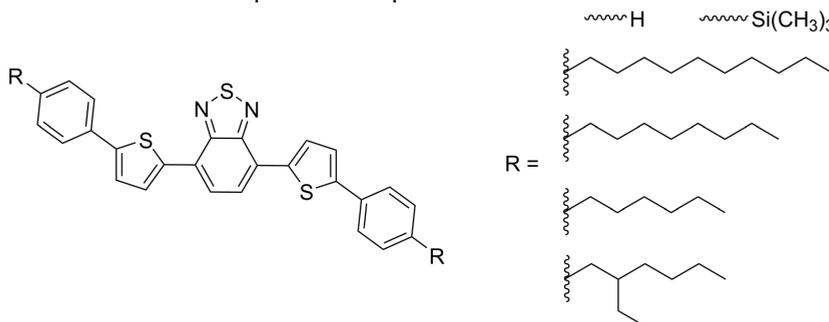


Fig. 1. Chemical structure of the obtained luminophores

In this study, a synthesis method was developed to create symmetrical luminescent molecules comprised of a BTD core as the electron-withdrawing component and thiophene and benzene moieties. This synthesis was accomplished through the direct arylation reaction. Additionally, molecules with various terminal substitutions, such as trimethylsilyl derivatives, as well as derivatives with hexyl, octyl, 2-ethylhexyl and decyl chains, were synthesized to examine their crystal packing behavior. The emission-luminescent properties of these derivatives in diluted solutions within tetrahydrofuran, as well as their thermal characteristics through differential scanning calorimetry and thermogravimetric analysis, were studied to assess the impact of the terminal groups.

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

<sup>1</sup> Skorotetcky 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.

<sup>2</sup> Postnikov V.A., Lyasnikova M.S., Kulishov A.A., Sorokina N.I., Voloshin A.E., Skorotetcky M.S., Borshchev O.V., Ponomarenko S.A. *Physics of the solid state*. 2019, **61**(12), 2322-2355.

## Synthesis of Organosilicon Copolymers with Grafted Biotin-Containing BTBT Segments

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Organic semiconductors (OSCs) have received considerable attention due to their exceptional optoelectronic properties in organic electronics, such as organic field-effect transistors (OFETs) and organic light-emitting diodes (OLEDs).

Among the various chemical structures used in low molecular OSCs, [1]benzothieno[3,2-b]benzothiophene (BTBT) represents a favorable core structure for high-performance OFETs.

Immobilization of biological receptors on the surface of organic semiconductors or gates by fixing molecules specific to the corresponding biomarkers facilitates binding to the target analyte and ensures the selectivity of the device.<sup>1</sup>

Currently, BTBT chemistry is being widely studied, with significant attention being paid to varying structural modifications to optimize solubility, crystallinity, and stability. In this regard, aliphatic units containing reactive chloraldehyde groups can react with the BTBT core, to effect the targeted introduction of alkyl chains at positions 2 and 7.<sup>2</sup>

BTBT derivatives were obtained through a multi-step procedure involving selective Friedel-Crafts acylation at the 2,7-position, reduction of corresponding ketogroups, and subsequent hydrosilylation reactions facilitated by Karstedt's catalyst. The integration of the biotin fragment was achieved by the azide-alkyne Huisgen cycloaddition, carried out in the presence of copper(I) ions.

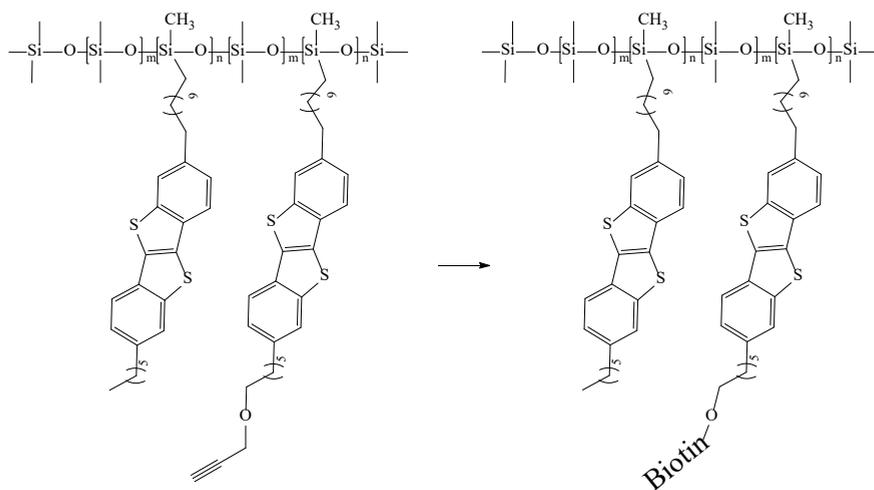


Fig. 1. Structural formulas of synthesized compounds

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

<sup>1</sup> Elena Yu. Poimanova et.al *ACS Appl. Mater. Interfaces* 2022, **14**, 16462–16476

<sup>2</sup> Ebata, Hideaki et.al *J. Am. Chem. Soc.* 2007, 129(51), 15732–15733

## Novel Luminophores Based on 2,1,3-Benzothiadiazole Containing Phenyl, Thiophene and Various Terminal Substituents

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Luminophores, as functional materials, are successfully used in various fields of science and technology. Among these materials, derivatives of 2,1,3-benzothiadiazole play a significant role due to their unique optical and electronic properties. The luminescent properties of these molecules can be tuned by incorporating different donor substituents.<sup>1</sup>

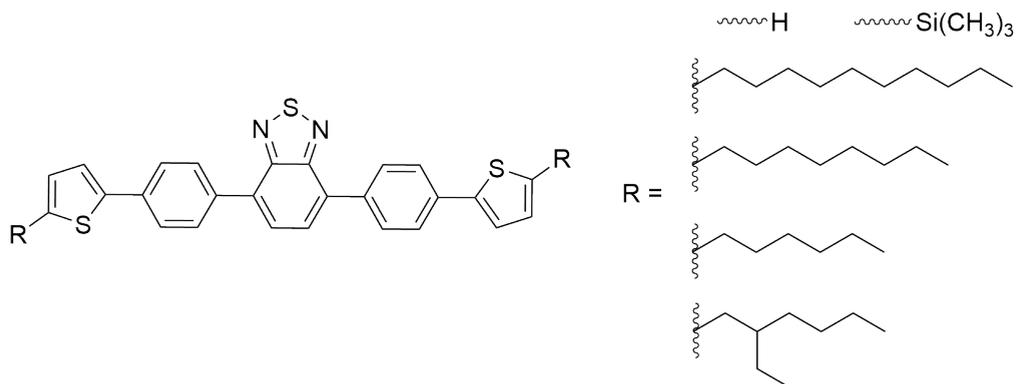


Fig. 1. Chemical structure of the obtained compounds

The main goal of this work is to investigate the relationship between the chemical structure and properties of these systems. A series of conjugated compounds based on 2,1,3-benzothiadiazole were synthesized, which contain donor thiophene and benzene moieties in their structures, as well as various terminal substituents. Optimal methods for obtaining these compounds through Pd-catalyzed cross-coupling reactions (Suzuki) were developed in two different ways. The spectral properties of the compounds obtained in dilute solutions were also investigated. The influence of alkyl substituents on the thermal properties was investigated using TGA/DSC techniques.

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

<sup>1</sup> Skorotetcky 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.

## Synthesis and Optoelectronic Properties of Thiophene-Containing Derivatives of Tris(2,4,6-Trichlorophenyl)methyl Radical

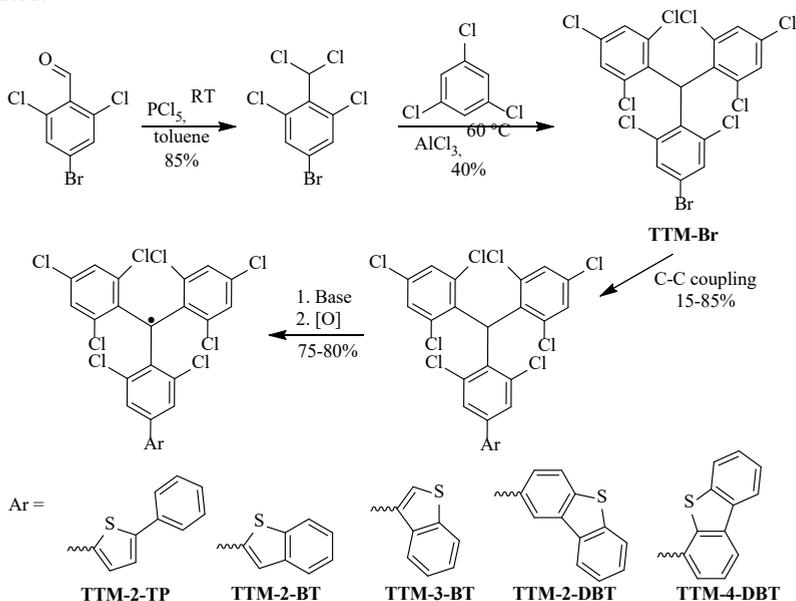
*E.D. Tolkachev*<sup>1\*</sup>, *C.S. Becker*<sup>1</sup>, *M.S. Kazantsev*<sup>1</sup>

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Organic luminophores are functional materials being attractive for practical applications in optoelectronic devices. Typically, these molecules have a singlet ground state with a closed-shell. However, in recent years, materials with an open-shell, such as organic luminescent radicals, have been gaining popularity due to the unique photophysical properties, the absence of heavy atom effects, the high efficiency OLEDs, as well as photoluminescence in the red and near IR regions.<sup>1</sup>

Tris(2,4,6-trichlorophenyl)methyl radical (TTM) was demonstrated to have distinct photoluminescence in solution at room temperature. At the same time, by modifying its structure with various substituents, it is possible to control its optoelectronic properties.<sup>2</sup> In this work, approaches to the synthesis of thiophene-containing derivatives of the TTM radical have been developed (Fig. 1), their optical properties have been studied, photoluminescence quantum yields in solution and films have been measured, and photostability in solution has been evaluated.



**Fig. 1.** Synthetic route for the thiophene-containing derivatives of the TTM radical.

*This work was supported by State Assignment of Ministry for Science and Higher Education of Russian Federation (FWUE-2022-0011).*

<sup>1</sup> Matsuoka R., Mizuno A., Mibu T., Kusamoto T. *Coord. Chem. Rev.* 2022, **467**, 214616.

<sup>2</sup> Velasco D., Castellanos S., López M., López-Calahorra F., Brillas E., Juliá L. *J. Org. Chem.* 2007, **72**, 20, 7523–7532.

## Experimental and Calculated Electronic Structure of Organic Semiconductors Based on BenzoThienoacene

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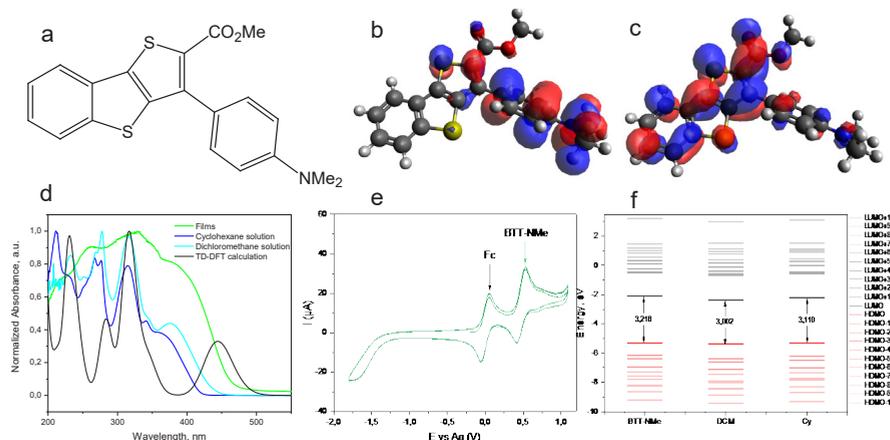
<sup>2</sup>Institute of Organic synthesis of Ural Branch of the Russian Academy of Sciences

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Investigating the properties of new compounds of semiconductor materials is of great interest in the field of design of various optoelectronic devices. Compounds derived from thiophenes are particularly promising due to their planar molecular structure, which facilitates a stable connection system and enables efficient charge transfer within the molecules.<sup>1,2</sup> The study focused on exploring the optical characteristics of semiconductor organic materials derived from benzo[b]thieno[2,3-d]thiophenes (BTT) featuring functional groups such as oxymethyl, oxyethyl, dimethylamine, benzene, and carboxylate, as well as carbonitrile groups (BTT-OMe, BTT-OEt, BTT-3,4OMe, BTT-2,5OMe, BTT-4OMe, B-BTT-3,4OMe, OMe-BTT-3,4OMe, BTT-NMe, BTT-2OMe, CN-BTT-OMe, BTT-Thio) in solution. This work utilized both experimental techniques and DFT calculations.

The ten compounds were studied in solutions of the polar solvent dichloromethane and the nonpolar cyclohexane with concentrations of 0.01  $\mu\text{mol L}^{-1}$ . Experimental and theoretical values of the energy of molecular orbitals and energy gap were determined using cyclic voltammetry, absorption optical spectroscopy and quantum chemical calculation (Fig. 1). The energy of HOMO and LUMO are in the range -5.1–6.2 eV and -3.5–2.3 eV, respectively, showing the influence of functional groups on charge transfer processes.

The report provides experimental and calculated data on the optical properties and electronic structure of the samples under study. The influence of functional groups on solubility, energy gap, and optical properties of BTT is discussed.



**Fig.1** Chemical structures of BTT-NMe (a), HOMO (b) and LUMO (c) visualization, absorbance spectra (d), cyclic voltammogram (e) and energy diagrams (f).

*This research funding from the Ministry of Science and Higher Education of the Russian Federation (Ural Federal University Program of Development within the Priority-2030 Program) is gratefully acknowledged.*

<sup>1</sup> K. Xiao, Y. Liu, T. Qi, at all, *J. Am. Chem. Soc.*, 2005, **127**, pp. 13281–13286.

<sup>2</sup> M. Wykes, B. Milián-Medina, J. Gierschner, *Front. Chem.*, 2013, **1**, 00035.

## Modeling the Charge Traps Influence on Organic Phototransistor Performance with Spatially Localized Photoelectric Effect

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Ambipolar organic field-effect transistors can exhibit spatially localized photoelectric effect (Fig. 1a). The electron-hole recombination zone in channel of such transistors can act as a photosensitive region where the maximum electric field is reached so that the photogenerated electron-hole pairs are efficiently separated. The position of the recombination zone in the channel can be controlled by the gate voltage,  $V_G$ , which makes such transistors promising for development of new devices, such as position sensing devices with high spatial resolution<sup>1</sup>. Using drift-diffusion numerical model, it was shown that the normalized photocurrent  $J_{ph}/J_{dark}$  dependences on  $V_G$  can reproduce the spatial profiles of incident light intensity across the phototransistor channel, after transformation of the  $V_G$ -scale to  $x$ -scale in accordance with the position dependence of the electric field peak on  $V_G$ <sup>2</sup>.

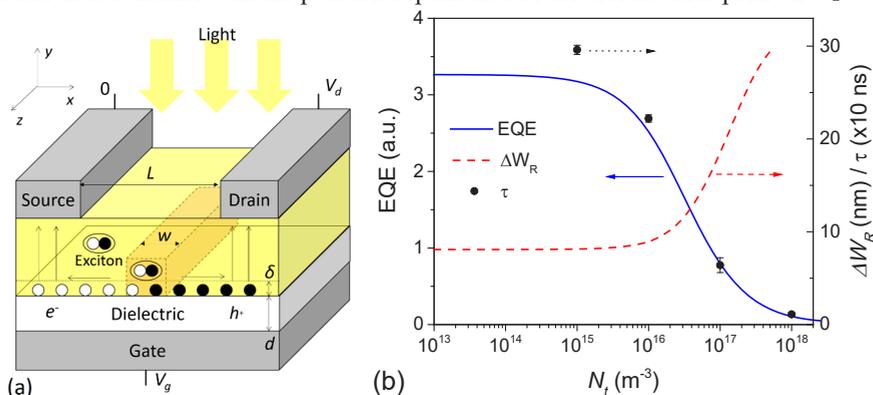


Fig. 1. Organic phototransistor scheme (a), dependences of the external quantum efficiency (EQE) (blue solid line, scale on the left), the parameter  $\Delta W_R$  characterizing the spatial resolution (red dashed line, scale on the right) and response time  $\tau$  (black dots, scale on the right) on the deep charge trap concentration  $N_t$  (b).

Organic semiconductors often contain impurities and defects which can act as charge traps. In current work the effect of deep and shallow charge traps on performance of organic phototransistor capable of spatially localized photoelectric effect is studied using numerical model. It was shown that the increase of deep charge trap concentration over  $10^{15} \text{ m}^{-3}$  makes the response time to turning on/off the incident illumination significantly faster, however EQE and spatial resolution become rather deteriorated. Also the effect of shallow traps which act as dopants on performance of phototransistor was studied and it was shown that near-contact doping can increase performance of phototransistor in case of non-Ohmic source/drain contacts. The results of numerical modeling obtained in current work can contribute to the development of novel organic optoelectronic devices with required characteristics.

*This work was supported by RSF (project № 22-79-10122).*

<sup>1</sup> D. Kabra, et al., *Appl. Phys. Lett.* 2004, **85**, 5073.

<sup>2</sup> V. A. Trukhanov, *Moscow Univ. Phys. Bull.* 2020, **75**, 342-353

## Synthesis and Properties of Novel Polysiloxanes Grafted with Dialkyl BTBT Derivatives

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Various derivatives of benzothieno[3,2-b][1]benzothiophene (BTBT) are widely used in OFETs due to their great properties. Among them are organosilicon derivatives of BTBT [1]These new materials combine, in addition to high charge carrier mobility, thermal and air stability and good solubility in common organic solvents.<sup>1</sup> 1,3-bis{11-(7-heptyl[1]benzothieno[3,2-b][1]benzothio-2-yl)hexyl}-1,1,3,3-tetramethyldisiloxane (D2-Hept-BTBT-Hex) was used in electrolyte-gated organic field-effect transistors to fabricate a virus biosensor.<sup>2</sup> In the work<sup>3</sup> series of D2-Und-BTBT derivatives and the influence of terminal alkyl fragments on the compound properties are reported.

Transition from disiloxane dimers to silicone polymers containing non-symmetric dialkyl BTBT derivatives as side chains could provide novel functional materials with good semiconducting and mechanical properties suitable for ink-jet printing. The first example of polymer materials containing 2-(undecyl-11-en)-7-hexyl[1]benzothieno[3,2-b][1]benzothiophene side chains grafted to polysiloxane main-chain (Px-Und-BTBT-Hex) were synthesized by the hydrosilylation of polymethylsiloxane matrices with varying ratio of functional methylsiloxane and nonfunctional dimethylsiloxane fragments.<sup>4</sup> It was shown that they have good thermal and thermo-oxidative stabilities, but form liquid crystalline mesophases only that does not favor to any good semiconducting properties. Only their mixtures with dioctyl-BTBT made it possible to measure reasonable field-effect mobility in OFETs.

In this work, similar siloxane polymer materials with longer (C8) terminal alkyl fragments (Px-Und-BTBT-Oct) were obtained and investigated by TGA and DSC in pure form as well as in their blends with dioctyl-BTBT. Thin films were deposited with blends and studied by atomic force microscopy (AFM). The results of their semiconducting properties investigation will be compared with those obtained with Px-Und-BTBT-Hex obtained previously.

*The work was carried out with the support of the Russian Science Foundation (project No. 19-73-30028).*

<sup>1</sup> Trul A.A., Chekusova V.P., Anisimov D.S., Borshchev O.V., Polinskaya M.S., Agina E.V., Ponomarenko S.A. *Adv. Electron. Mater.* 2022, **8**, 2101039.

<sup>2</sup> Poimanova E.Y., Zavyalova E.G., Kretova E.A., Abramov A.A., Trul A.A., Borshchev O.V., Keshchek A.K., Ponomarenko S.A., Agina E.V. *Chemosensors* 2023, **11**(8), 464.

<sup>3</sup> Polinskaya M.S., Trul A.A., Borshchev O.V., Skorotetsky M.S., Gaidarzhi V.P., Toirov S.K., Anisimov D.S., Bakirov A.V., Chvalun S.N., Agina E.V., Ponomarenko S.A. *J. Mater. Chem. C*, 2023, **11**, 1937.

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## Triphenylamine-based Push-pull Small Molecules As A Platform For Elaborating Organic Semiconductor Materials With A Wide Applications Range

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The elaboration and molecular design of novel organic semiconducting materials, as well as their use as an element base for the development of electronic and optoelectronic devices, has become an actively growing and economically justifiable area of fundamental and applied research over the past decade. Conjugated donor-acceptor organic materials have become an important class of such materials owing to their unique combination of optical and electronic properties and wide potential applications in organic electronic devices, and other fields of science and technology.

Herein, we report on synthesis and comprehensive investigation of the different series of novel push-pull molecules with triphenylamine unit as an electron donor block, which end-capped with various types of electron-withdrawing groups, in particular, functional groups. The analysis of the results obtained made it possible to establish a number of significant structurally inherent regularities and to suggest possible areas of their application, for example, as effective photoconversion coatings, organic phosphors, functional photoactive and auxiliary layers of organic and hybrid photonics. Depending on the group nature different optical properties, for example, luminescence maxima of the luminophores demonstrated significant variability, *e.g.* from 509 nm to 750 nm, while the photoluminescence quantum yield values laid in the range of 1–89%. Some materials were found to be good compatibility with a polymer matrix, in which photoluminescence quantum yields were generally higher (up to 25-fold enhancement) compared to the corresponding solutions or polycrystalline films.

*This work was supported by the Russian Science Foundation (project № 23-73-01278).*

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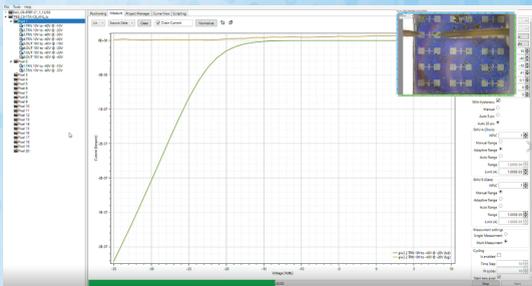
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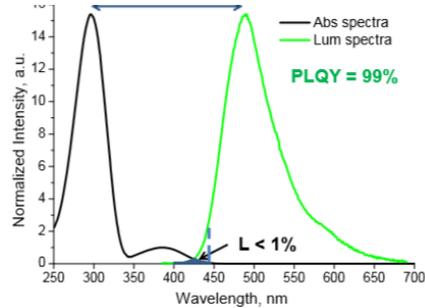
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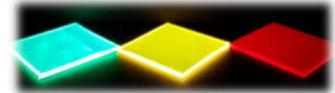
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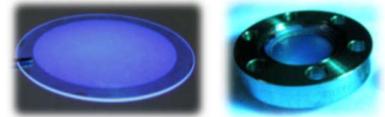
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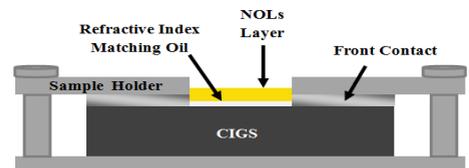
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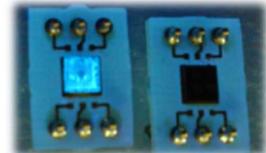
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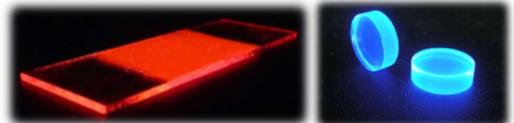
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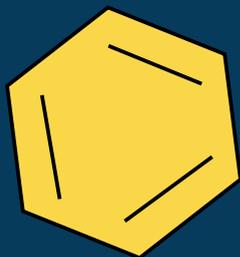
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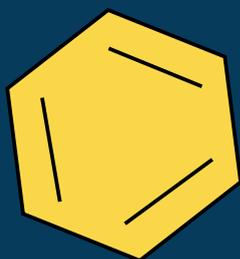


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