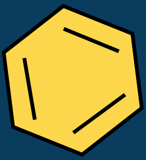
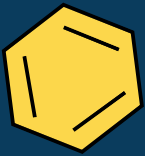
IFSOE
2021



7th International Fall School on Organic Electronics

Book of Abstracts



September 13-16, 2021
Moscow, Russia
ISPM RAS
http://www.ifsoe.ru

7th INTERNATIONAL FALL SCHOOL ON ORGANIC ELECTRONICS – 2021 (IFSOE-2021)

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)

Printed Electronics Technologies Limited Liability Company (PrintElTech LLC)

Eklogit Limited Liability Company (Eklogit LLC)

Scientific program

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

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

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

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

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

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

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

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

School-conference Chairs

Prof. Sergey Ponomarenko (Enikolopov Institute of Synthetic Polymeric Materials of RAS, Russia)

Prof. Dmitry Paraschuk (Lomonosov Moscow State University, Russia)

International Advisory Board

Prof. Vladimir Agranovich (Institute for Spectroscopy RAS, Russia)
Prof. Mikhail Alfimov (Photochemistry Center of RAS, Russia)
Prof. Paul Berger (Ohio State University, USA)
Prof. Christoph Brabec (University Erlangen-Nürnberg, Germany)
Prof. Sergei Chvalun (National Research Center "Kurchatov Institute", Russia)
Prof. Vladimir Dyakonov (University of Würzburg, Germany)
Prof. Antonio Facchetti (Northwestern University, USA)
Prof. Sir Richard Friend (University of Cambridge, UK)
Prof. Marcus Halik (University Erlangen-Nürnberg, Germany)
Dr. Stephan Kirchmeyer (Heraeus Precious Metals GmbH, Germany)
Prof. Alexei Khokhlov (Lomonosov Moscow State University, Russia)
Prof. Guglielmo Lanzani (Politechnico di Milano, Italy)
Prof. Maxim Pshenichnikov (University of Groningen, the Netherlands)
Dr. Abderrahim Yassar (Ecole Polytechnique, France)

Local Organizing Committee

Dr. Elena Agina – *Vice Chairman*
Victoria Chekusova – *workshop secretary*
Dr. Askold Trul
Daniil Anisimov
Polina Shaposhnik

Book of abstracts. 7th International Fall School on Organic Electronics – 2021 (IFSOE-2021) // Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences. - Moscow, 2021. - 100 pages.

ISBN 978-5-6043936-2-8.

ISBN 978-5-6043936-2-8

9 785604 393628

School program

The 7th International Fall School on Organic Electronics – 2021 Time Schedule

Moscow, Russia (GMT+3)

	Monday *September 13th*	**Tuesday** *September 14th*	**Wednesday** *September 15th*	**Thursday** *September 16th*
	School			
9:45-10:00	**School opening**			
10:00	**Paul Blom**	**Magnus Berggren**	**Ronald Resel**	**Paolo Samori**
11:00	**Dmitry Paraschuk**	**Luisa Torsi**	**Sergey Ponomarenko**	**Deiter Neher**
12:00	**Coffee-break**			
	Valentina Utochnikova	**Alexandra Freidzon**	**Sandrine Heutz**	**Ivan Scheblykin**
13:00	Oral talks 1	Oral talks 2	**Jie Min**	Oral talks 5
14:00			Oral talks 4	
	Lunch			**School closing**
15:00				
16:00	Poster session 1	Oral talks 3	Poster session 3	
		Poster session 2		
17:00	**Welcome-party**		**Conference Dinner**	

Monday, September 13th

	Chair: *Sergey Ponomarenko*
9:45 – 10:00	**School opening**
10:00 – 11:00	**T-1**. *Paul Blom.* Electron and Hole Transport in Organic Semiconductors
11:00 – 12:00	**T-2**. *Dmitry Paraschuk.* Organic Light Emitting Transistors

12:00 – 12:30	**Coffee-break**
	Chair: *Paul Blom*
12:30 – 13:00	**I-1**. *Valentina Utochnikova.* Lanthanide Complexes as OLED Emission Layers
	Oral talks 1.
13:00 – 13:15	**O-1**. *Maxim Kazantsev.* Selectively Fluorinated Furan-Phenylene Co-Oligomers for Light-Emitting Transistors
13:15 – 13:30	**O-2**. *Koskin Igor.* Furan-Phenylene Co-Oligomers: Theoretical Modelling Paves Way for the Molecular Smart-Design
13:30 – 13:45	**O-3**. *Makarii Kozlov.* Methods for Reducing the Lifetime of the Excited State to Increase the Efficiency of Lanthanide-Based OLEDs
13:45 – 14:00	**O-4**. *Kostas Daoulas.* Mesoscopic Modeling of Disordered Morphologies of Blends and Block-Copolymers for Application in Light Emitting Diodes
14:00 – 14:15	**O-5**. *Sergey Tokarev.* Modification of the Carrier Mobility of Conducting PF-EP Polymer by Doping with Thiophene Derivatives
14:15 – 14:30	**O-6**. *Andrey Kornikov.* Ytterbium-Europium Dibenzoylmethanates with Bathophenanthroline in OLEDs
14:30 – 15:30	**Lunch**
	Chair: *Yuriy Luponosov*
15:30 – 16:40	**Poster session 1 (*P-1 – P-14*)**
16:40 – 17:00	**Discussion regarding to Poster session 1**
17:00 – 18:00	**Welcome-party**

Tuesday, September 14th

	Chair: *Elena Agina*
10:00 – 11:00	**T-3**. *Magnus Berggren.* P- and n-type Conducting Polymers for Bioelectronic and Internet-of-Things Applications
11:00 – 12:00	**T-4**. *Luisa Torsi.* Bioelectronic Single-Molecule Label-Free Sensing with Large-Area Transducing Interfaces
12:00 – 12:30	**Coffee-break**
	Chair: *Luisa Torsi*
12:30 – 13:00	**I-2**. *Alexandra Freidzon.* Theoretical Prediction of Charge Mobility in Molecular Organic Semiconductors
	Oral talks 2.
13:00 – 13:15	**O-7**. *Oleg Kharlanov.* Spectroscopic Assessment of Charge-Carrier Mobility in Organic Semiconductors

13:15 – 13:30	**O-8**. *Konstantin Ivanov.* Spiroconjugation Effect on Optoelectronic Properties of Spirobi[indene]-1,1’(3H,3’H)-diones with Extended Conjugation
13:30 – 13:45	**O-9**. *Sergey Novikov.* Density of States in Locally Ordered Amorphous Organic Semiconductors: Emergence of the Exponential Tails
13:45 – 14:00	**O-10**. *Vladimir Nikitenko.* Off-Diagonal Disorder and Field-Assisted Diffusion in Disordered Organic Semiconductors
14:00 – 14:15	**O-11**. *Roman Peshkov.* DFT Benchmark of Geometry and Excited States of Spiro[4,4]nona-1,3,6,8-tetraene
14:15 – 14:30	**O-12**. *Rishabh Saxena.* Role of the Reorganization Energy for Charge Transport in Disordered Semiconductors
14:30 – 15:30	**Lunch**
	Oral talks 3. Chair: *Oleg Borshchev*
15:30 – 15:45	**O-13**. *Daniil Anisimov.* The Mechanism for Changing the Organic Field-Effect Transistors (OFETs) Electrical Properties of under Toxic Gases Exposure
15:45 – 16:00	**O-14**. *Alexandra Zvyagina.* Self-Assembly of Recyclable Supramolecular 1D Semiconductors from bis-Phthalocyanines on Solid Surfaces
16:00 – 16:15	**O-15**. *Yuriy Luponosov.* Liquid Luminophores Based on Organic π-conjugated Oligomers with Alkylsilyl Solubilizing Groups
16:15 – 16:30	**O-16**. *Alexey Kuevda.* Enhancement of Light-Emitting Properties of 2D Organic Semiconductors via Molecular Doping
16:30 – 17:15	**Poster session 2** (***P-15 – P-23***)
17:15 – 17:30	**Discussion regarding to Poster session 2**

Wednesday, September 15th

	Chair: *Dieter Neher*
10:00 – 11:00	**T-5**. *Roland Resel.* Thin Film Structure by X-ray Scattering Methods: The Example of an Assymetric BTBT Derivative
11:00 – 12:00	**T-6**. *Sergey Ponomarenko.* Gas Sensing with Organic Electronics: from Single Sensors to Electronic Nose
12:00 – 12:30	**Coffee-break**
	Chair: *Roland Resel*
12:30 – 13:30	**T-7**. *Sandrine Heutz.* Molecular Magnetic Semiconductor Thin Films for Spintronic Applications
13:30 – 14:00	**I-3**. *Jie Min.* Balancing the Efficiency, Stability, and Cost Potential for Organic Solar Cells via a New Figure of Merit
	Oral talks 4.

14:00 – 14:15	**O-17**. *Rinat Salikov.* Cascade Reactions in Seven-Membered Systems: Towards Innovative Functional Materials
14:15 – 14:30	**Sponsor talk.** *Michael Trusov.* Imaging Ellipsometry and Near-field Microscopy Techniques for Organic Electronics Applications
14:30 – 15:30	**Lunch**
	Chair: *Andrey Sosorev*
15:30 – 17:05	**Poster session 3 (*P-24 – P-41*)**
17:05 – 17:30	**Discussion regarding to Poster session 3**
17:30 – 21:00	**Conference Dinner**

Thursday, September 16th

	Chair: *Ivan Scheblykin*
10:00 – 11:00	**T-8**. *Paolo Samori.* Multifunctional Organic Electronics
11:00 – 12:00	**T-9**. *Dieter Neher.* Organic Solar Cells – On the Generation and Fate of Free Carriers
12:00 – 12:30	**Coffee-break**
	Chair: *Dmitry Paraschuk*
12:30 – 13:00	**I-4**. *Ivan Scheblykin.* Luminescence Spectroscopy and Microscopy for Conjugated Polymers
	Oral talks 5.
13:00 – 13:15	**O-18**. *Alexei Komolov.* Conduction Band Energy Profile and Surface Work Function of Vacuum Evaporated Molecular Films on Binary Semiconductor Surfaces
13:15 – 13:30	**O-19**. *Artur Mannanov.* Effect of Oligothiophene π-bridge Length in D-π-A Star-Shaped Oligomers on Photophysics and Photovoltaic Performance in Organic Solar Cells
13:30 – 13:45	**O-20**. *Pavel Komarov.* Mesoscale Simulations of Photovoltaic Polymer Nanocomposites
13:45 – 14:00	**O-21**. *Maxim Skorotetcky.* Synthesis and Properties of Thienoacenes for Organic Electronics
14:00 – 14:15	**O-22**. *Elizaveta Gusarova.* Ultrathin Hybrid Surface Coatings from Graphene Oxide and Polydiacetylenes for Fabricating Organic Photodiodes
14:15 – 14:30	**O-23**. *Ben Carwithen.* Hot Carrier Cooling Dynamics in Lead Halide Perovskite Nanocrystals Revealed by Ultrafast Multi-Pulse Spectroscopy
14:30 – 15:00	**School closing**

Poster session 1

Monday, September 13th, 15:30

Abramov, Anton A.	P1	Compact Hardware Platform for Multiple Electrochemical and Metal-Oxide Sensors Evaluation
Balakirev, Dmitry O.	P2	Novel Thiophene-Containing Donor Small Molecules With Various Topology: Synthesis, Properties and Application in Organic Solar Cells
Borshchev, Oleg V.	P3	New Organic Luminophores for Optoelectronics
Bujaldon, Roger	P4	Tuning the Optoelectronic Properties of Sulfurated Carbazole Derivatives: the Case of the Bisbenzothienocarbazole Core
Burdakov, Yaroslav V.	P5	Modelling of Charge Transport in Polymers with Imbedded High-Ordered Nanoscale Regions
Chukhlantseva, Anna N.	P6	Novel Chalcones Containing 4-bis(2-hydroxyethyl)aminophenyl Moiety: Synthesis and Optical Properties.
Chuyko, Irina A.	P7	Novel Donor-Acceptor Triphenylamine-Based Polymer for Organic and Hybrid Electronics
Dyadishchev, Ivan V.	P8	Synthesis and Properties of Novel Liquid Luminescent Chromophores Based on Organic π-Conjugated Oligomers
Fedorenko, Roman S.	P9	Effect of Molecular Doping on Charge Transport and Electroluminescence of 2D Organic Semiconductors
Kuklin, Konstantin N.	P10	Impact of the Chemical Purity on the Semiconductor Properties of 2D Single Crystals
Kalinichenko, Nadezhda K.	P11	Synthesis of Novel Donor-Acceptor Triazatruxene-Based Isomers End-Capped with Alkyldicyanovinyl or Cyanoacetate Groups
Khmelnitskaya, Alina G.	P12	A New Approach for Obtaining Functional Dimethylsiloxane Matrices for Dielectric Elastomer Actuators
Kleymyuk, Elena A.	P13	Copolymers Based on Polyvinylidene Fluoride and Chlorotrifluoroethylene with Grafted Polyacrylonitrile or Poly (Ethyl Methacrylate) Chains for Ferroelectric Organic Field-Effect Transistors
Kobeleva, Elena S.	P14	Origin of Poor Photovoltaic Performance of Bis(tetracyanoantrathiophene) Non-Fullerene Acceptor

Poster session 2

Tuesday, September 14th, 16:30

Kuimov, Anatolii	P15	Optical Properties of Selectively Fluorinated Furan-Phenylene Co-Oligomers
Martynov, Ilya V.	P16	Towards Understanding the Chemical Structure - Oxidation Stability Relationships for Conjugated Polymers used in Organic Solar Cells
Moshkina, Tatiana N.	P17	V-Shaped Chromophores Based on Quinoxaline and Cyclopenta[c] pyridine: Synthesis and Perspective Applications
Poimanova, Elena Yu.	P18	A New Approach for Fabrication of Biorecognition Layer in Electrolyte-Gated Organic Field-Effect Transistors

Polinskaya, Marina S.	P19	Synthesis and Properties of New Organosilicon Derivatives of [1] benzotieno[3,2-b][1] - benzothiophene with Different Length of Terminal Aliphatic Substituents
Sachkov, Yuri I.	P20	Conductivity of Solution-Processed Thin Films of Chlorophyll Derivatives: Drop-Casting vs. Spin Coating
Koshelev, Daniil S.	P21	Lanthanide Complexes with 2-(tosylamino)-benzylidene-N-(aryloyl)-hydrazones in NIR OLEDs
Kuznetsov, Kirill M.	P22	Europium β-Diketonates with Dipyrido [3,2-a:2′,3′-c] Phenazine in OLED
Obukhov, Alexandr E.	P23	Organic Electronic and the Orbital Properties Singlets, Triplets, Duplets, Quartets Electronic Excited States in the Series Multiatomic Compounds of Fluorescence and Generation of Dye-Lasers

Poster session 3

Wednesday, September 15th, 15:30

Bezsudnov, Igor V.	P24	Rejuvenation of Two-Phase Composite Employing Liquid-Gas Phase Transition Using Different Solvents
Chekusova, Victoria P.	P25	Fabrication of the Patterned Polymer Substrates for Fully Printed Polymer OFETs Creation
Samburskiy, Denis E.	P26	Carbazole-Decorated Spiroconjugated Pure Organic Phosphorescent Materials Based on 2,2'-spirobi[indene] and 5,5'-spirobi[cyclopenta[b]thiophene] Linkers
Saunina, Anna Yu.	P27	Physical Modeling of the Charge and Excitation Transport in QD-Based and Hybrid Photovoltaic Cells
Konstantinov, Vladislav G.	P28	Method for Estimating the Photoluminescence Quantum Yield of Extremely Thin Organic Crystals
Saxena, Rishabh	P29	Role of the reorganization energy for charge transport in disordered semiconductors
Shaposhnik, Polina A.	P30	A Study on Stability of Electrolyte-Gated Transistor Based on 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene Blends with Polystyrene
Shumilov, Nikita A.	P31	Charge Transport in Single Crystals of 1,4-bis(5-phenylfuran-2-yl) Benzene and its Fluorinated Derivatives
Solodukhin, Aleksandr N.	P32	Triphenylamine-Based Small Molecules for Pixelated Full-Colour Semiconductor Devices Towards Artificial Retinas
Sonina, Alina A.	P33	Crystal Structure of Selectively Fluorinated Furan-Phenylene Co-Oligomers
Sosorev , Andrey Yu.	P34	Charge Transport Highways Within Ribosomal Small Subunit
Titova, Yaroslava O.	P35	Inkjet Printing of Organic Electrochemical Transistors with PEDOT:PSS Ink
Trainov, Konstantin P.	P36	Synthesis of Chromophores Based on the Hydrazinylidene Cyclic Acceptor Moieties via the Reaction of Organolithium Reagents with Diazo Compounds
Trukhanov, Vasiliy A.	P37	Electroluminescence Polarization Anisotropy in Organic Semiconductor Crystals

Trul, Askold A.	P38	Ethanethiol Detection with Operationally Stable Ultrathin BTBT-Dimers-Based OFETs
Yang, Wenchao	P39	Kinetic Monte Carlo Simulation of Exciton Dynamics in Non-Fullerene Acceptor Solar Cells
Zaborin, Evgeniy A.	P40	Synthesis and Properties of the New Linear Polymers Based on Annelated Structures
Ghosh, Sanjay S.	P41	Application of Solvents and Solvent Mixtures to Control the Bulk-Heterojunction Morphology
Shepovalov, Kirill M.	P42	Optelectronic Properties of Spiro[4.4]nonatetraen Based Hydrocarbons

Tutorial lectures

Electron and Hole Transport in Organic Semiconductors

P. Blom[1*], *N. Kotadiya*[1], *A. Mordan*[1], *D. Andrienko*[1], *G.-J. Wetzelear*[1]

[1]Max Planck Institute for Polymer Research
**e-mail: blom@mpip-mainz.mpg.de*

Organic semiconductors are used in optoelectronic devices, such as organic light-emitting diodes, organic and perovskite solar cells, and organic field-effect transistors. The performance of such devices depends heavily on charge injection and transport. In many cases, organic semiconductors exhibit highly unipolar charge transport, meaning that they predominantly conduct either electrons or holes. A fundamental question is what causes this unipolarity. We demonstrate that an energetic window exists inside which organic semiconductors are not susceptible to charge trapping by water or oxygen, leading to trap-free charge transport of both carriers. The implication for devices such as OLEDs, organic solar cells and organic ambipolar transistors is that the energy levels of the organic semiconductors are ideally situated within this energetic window. However, for blue-emitting OLEDs with a large band gap this poses significant challenge to remove or disable charge traps.

T-2

Organic Light-Emitting Transistors

D.Yu. Paraschuk[1,2*]
[1]Faculty of Physics, Lomonosov Moscow State University
[2]Enikolopov Institute of Synthetic Polymeric Materials, Russian Academy of Science
*e-mail: paras@physics.msu.ru

Organic light-emitting transistor (OLET) — one of the "youngest" organic electronics devices — has a number of advantages over the more traditional organic light-emitting diodes (OLEDs), which are already widely used in displays of portable devices and advanced TV screens. For example, OLET can be much brighter, and the light can be outcoupled from it much more efficiently. Moreover, OLETs are the most promising platform for injection organic lasers, which have still to be demonstrated. In this tutorial, we review basics of OLETs, analyze the state of the art of the field, discuss the hurdles of correct OLET characterization, and present an outlook on the OLET future. Considering that one of the key bottlenecks in OLETs is their low efficiency, we introduce our vision of efficient OLETs that are based on 2D single crystals.

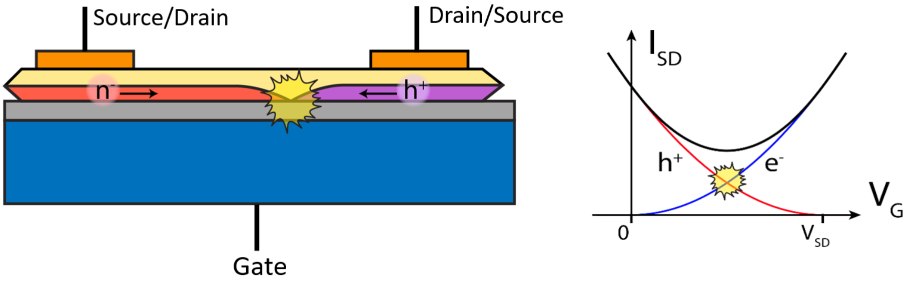


Figure 1. Schematic of OLET (left) and its transfer characteristic (right).

An ideal OLET is *per se* an ambipolar organic field-effect transistor (OFET) with a totally emissive active layer and Ohmic contacts (Figure 1). Taking in account that the charge transport in OFETs occurs within a few semiconductor monolayers adjacent to the semiconductor-dielectric interface, a perfect OLET active layer would be a molecularly thin (2D) single crystal of a brightly luminescent ambipolar semiconductor. 2D organic semiconductor single crystals of high structural quality are available now.[1] The high structural quality of semiconductor single crystals provides their superior electrical performance, and the 2D active layer is very beneficial for OLET to get rid of waveguiding effects that reduce the light output from thin film and 3D-single-crystal devices. However, combination of bright luminescence and efficient ambipolar charge transport in one material is a challenge, and we review promising materials for single-layer OLETs, specifically, thiophene-phenylene and furan-phenylene co-oligomers.[2,3] One of the key metrics of OLETs it their external quantum efficiency, and we discuss how to accurately evaluate it.

This work was supported by RFBR (project № 18-12-00499).

---

[1] Bruevich V.V. et al. *ACS Appl. Mater. Interfaces*, 2019, **11**, 7

[2] Borshchev O.V. et al. Dyes and Pigments 2021, **185**, 108911.

[3] Koskin I. P. et al. *Adv. Funct. Mater.,* 2021, 2104638 (published on-line).

P- and n-type Conducting Polymers for Bioelectronic and Internet-of-Things Applications

M. Berggren[1]

[1] Linkoping University

Bioelectronic Single-Molecule Label-Free Sensing with Large-Area Transducing Interfaces

L. Torsi[1*]

[1]Universita degli Studi di Bari Aldo Moro
*e-mail: luisa.torsi@uniba.it

Nanosized bioelectronic detecting interfaces seem the privileged pathway to single-molecule detections. However, while giving access to rarer events, this near-field approach is unsuited to detect at concentrations lower than nanomolar because of the diffusion-barrier issue. Large-area (μm^2 - mm^2 wide) bioelectronic transistors are perceived as unsuited due to the irrelevant footprint of a single molecule on a much larger detecting interface. *Indeed, it is like seeing the surface of a one-kilometer-wide pond that changes because a single droplet of water falls on it.* However, many field-effect large-area biosensors have been shown to detect at limit-of-detection below femtomolar, being also naturally suited for point-of-care applications. In this lecture the field will be discussed, illustrating device architectures, materials used, and target analytes that can be selectively detected. The sensing mechanisms and the amplification effects enabling the large-area bioelectronic sensor to detect at the physical limit are also detailed.

Thin Film Structure by X-ray Scattering Methods: The Example of an Assymetric BTBT Derivative

R. Resel[1]*

[1]Institute of Solid State Physics, Graz University of Technology, Austria
*e-mail: roland.resel@tugraz.at

The molecular class of benzo-thieno-benzothiophene (BTBT) has gained a lot of interest, since excellent performance is observed in thin film transistors. A further improve of the performance is obtained by using different types of side groups at the terminal ends of the BTBT core with a phenyl group (Ph) on one side and a decyl group (10) on the other side.[1] The resulting molecule Ph-BTBT-10 has an asymmetric molecular shape, it crystallises in a double layer herringbone structure with head-to-head arrangement of the molecules (see Figure left). The assymmetric nature of the molecule causes considerable differences in the crystallisation kinetics in comparison to semiconducting molecules with symmetric molecular shape.

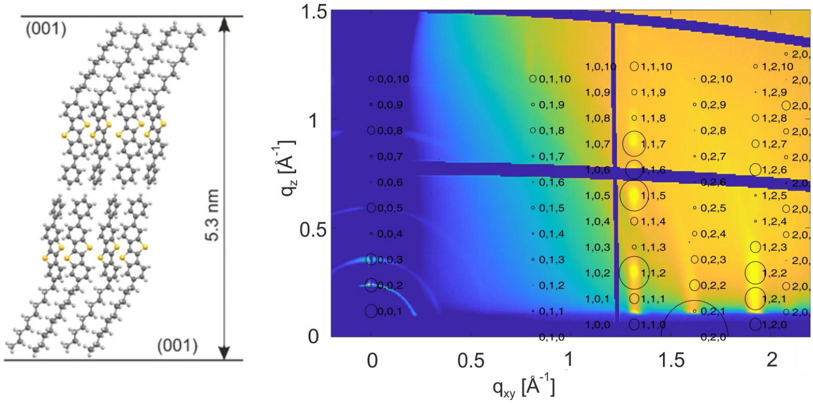


Fig. 1. Molecular Packing of the asymmetric molecule Ph-BTBT-10 within the crystal structure (left) and the corresponding reciprocal space map measured by grazing incidence X-ray diffraction (right)

We investigated the phase behaviour of this molecule and solved the molecular packing within the crystal / smectic E phase.[2] We investigated the thin film growth kinetics as a function of the film thickness by X-ray reflectivity combined with atomic force microscopy. An unknown thin film polymorph was found and solved using a combined experimental / theoretical approach. Additionally, an unusual broadening of the X-ray diffraction peaks is observed, which could be related to defects in the molecular packing of Ph-BTBT-10.[3] Finally, thin film transistors were prepared by bar assisted shear coating which reveal the anisotropy of the charge transport.[4] The tutorial lecture gives an introduction to X-ray based methods for the characterization of thin films used in organic electronic devices.

This work was supported by the Austrian Science Foundation (project № P30222).

---

[1] Ino, H., et al., *Nature Comm.* 2015, **6,** 6828.

[2] Hofer S, et al., *Liquid Crystals* 2021, **in press**.

[3] Hofer S, et al., *Chem. Mater.* 2021, **33,** 1455−1461.

[4] Tamayo, A., et al., *J. Mater. Chem. C* 2021, **9 (22)**, 7186–7193.

T-6

Gas Sensing with Organic Electronics: from Single Sensors to Electronic Nose

S.A. Ponomarenko[1,2*]

[1]Institute of Synthetic Polymer Materials RAS
[2]Moscow State University, Department of Chemistry
*e-mail: ponomarenko@ispm.ru

In this tutorial lecture a historical overview of gas sensors based on various conjugated oligomers and polymers will be presented. Key characteristics of the gas sensors, their main types, advantages and disadvantages will be discussed. Methods of sensory layers formation as well as possible ways for increasing their sensitivity and selectivity will be considered. Different mechanisms of sensory response will be described. The main focus of the lecture will be on the gas sensors based on organic field-effect transistors (OFETs) due to their outstanding sensitivities, low cost and small power consumption. It will be illustrated by the development of highly efficient monolayer OFETs for ultrasensitive gas sensors and electronic nose based on them. Since the first report on a monolayer OFET gas sensor based on self-assembly of very active chlorosilane derivative of quinquethiophene from solution[1], a great progress was achieved in fast deposition of the monolayers of highly stable disiloxane derivatives of BTBT (Figure 1, top)[2]. These monolayers have been successfully used in OFET gas sensors both with and without receptor layers[3,4]. Recently the first fully integrated OFET-based electronic nose with the whole sensor array located on a single substrate was reported (Figgure 1, left)[5]. By means of various machine learning algorithms (Figure 1, right), it is able to discriminate toxic air pollutants and even monitor meat freshness. This universal platform paves the way for developing affordable air sensing networks for process control, environmental monitoring, exhaled breath analysis and the Internet of Things.

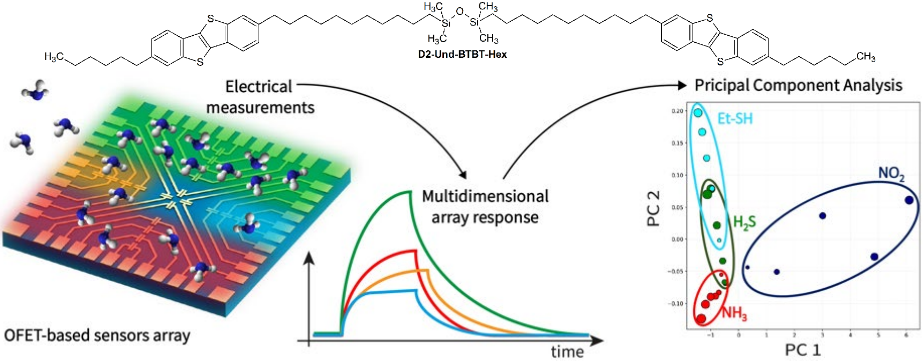


Figure 1. Chemical structure of the self-assembling organic semiconductor used (top) and a sketch of the OFET-based sensors array under exposure to NH3 molecules (left), its multidimentional array response (middle) and results of its analysis by PCA algorithm (right).

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

---

[1] Andringa, A.-M. M.-J. Spijkman, E.C.P. Smits, et al. *Org. Electron*. 2010, **11**, 895–898.
[2] O.V. Borshchev, A.S. Sizov, E.V. Agina, et al. *Chem. Comm*., 2017, **53**, 885-888.
[3] A.S. Sizov, A.A. Trul, V.P. Chekusova, O.V. Borshchev, A.A. Vasiliev, E.V. Agina, S.A. Ponomarenko, *ACS Appl. Mater. Interfaces*, 2018, **10**(50), 43831–43841
[4] A.A. Trul, V.P. Chekusova, M.S. Polinskaya, A.N. Kiselev, E.V. Agina, S.A. Ponomarenko, *Sensors and Actuators B: Chemical*, 2020, **321**, 128609
[5] Anisimov D.S., Chekusova V.P., Trul A.A., Abramov A.A., Borshchev O.V., Agina E.V., Ponomarenko S.A. *Sci. Rep.* 2021, **11**, 10683.

Molecular Magnetic Semiconductor Thin Films for Spintronic Applications

Z. Wu[1,2†]*, P. Robaschik*[1,2]*, D. Soukeras*[1,2]*, H. Demetriou*[1,2]*, H.H. Tseng*[1,2]*, L. R. Fleet*[1,2]*, S. Felton*[3]*, A. J. Fisher,*[4] *N. M. Harrison,*[5] *W. Wu,*[1,2] *G. Aeppli*[6]*, S. Heutz*[1,2*]

[1]Department of Materials, Imperial College London.
[2] London Centre for Nanotechnology, Imperial College London.
[2]School of Mathematics and Physics, Queen's University Belfast.
[4]Department of Physics and London Centre for Nanotechnology, University College London.
[5]Department of Chemistry, Imperial College London.
[6]ETH Zürich, EPF Lausanne and Paul Sherrer Institute.
† Current address: School of Physics, Dalian University of Technology.
*e-mail: s.heutz@imperial.ac.uk

Molecular materials present exciting advantages for spintronics and quantum technologies, due to their long spin-lifetime, and ability to incorporate multiple degrees of freedom, combining semiconductor behavior with the presence of a free spin.[1,2,3]

In this tutorial, some key concepts in spintronics will be presented, centred on the building block of spin-based logic, the spin valve. This device is traditionally based on inorganic materials but molecular thin films have been investigated as a relatively passive "spacer layer" that decouples the inorganic magnetic layers while maintaining spin coherence.[4] Further advances on this concept hinge on the creation of organic magnetic layers, and this presentation will review molecular magnetic materials, and the strategies to increase magnetic coupling.

In particular, the ability to grow (ferro)magnetic semiconducting molecular thin films on flexible substrates will be presented. The case study will focus on phthalocyanines (Pcs), polyaromatic molecules with a proven track record in solar cell research. By treating the substrates with a molecular template, the films can be oriented, harnessing their strong magnetic anisotropy, as well as tuning their Curie temperature.[5]

In the final part of the presentation, the utilization of the molecular spins for applications in quantum computing[6] will be reviewed, highlighting the specific advantages of organic frameworks over inorganic counterparts.

This work was supported by EPSRC (grant no EP/F039948/1; EP/F04139X/1).

---

[1] Atzori & Sessoli, *J. Am. Chem. Soc.* 2019, **141**,11339.
[2] Sanvito. *Chem. Soc. Rev.* 2011, **40**, 3336.
[3] Dediu *et al. Nat. Mater.* 2009, **8**, 707.
[4] Xiong, *et al. Nature* 2004, **427**, 821.
[5] Wu *et al. Adv. Funct. Mater.* 2019, **29**, 1902550.
[6] Gaita-Ariño *et al. Nat. Chem.* 2019, **11,** 301.

T-8

Multifunctional Organic Electronics

P. Samorì[1*]

[1]ISIS, Université de Strasbourg & CNRS
*e-mail: samori@unistra.fr

The development of multifunctional devices capable to respond to multiple and independent stimuli is one among the grand challenges in organic electronics. The combination of multiple components, with each one conferring a specific function to the ensemble, is a facile strategy to impart a multifunctional nature to electronic devices. The controlled combination of such components and their integration in real devices can be achieved by mastering the supramolecular approach.

In my lecture I will review our recent works on the combination of carbon-based nanomaterials, in particular comprising organic semiconductors, with photochromic molecules (diarylethenes or azobenzenes), in order to fabricate smart, high-performing and light-sensitive (opto)electronic devices such as field-effect transistors and light-emitting transistors and as well as flexible non-volatile optical memory thin-film transistor device with over 256 distinct levels.

---

[1] For reviews see: (a) X. Zhang, L. Hou, P. Samorì, *Nat. Commun.* 2016, **7**, 11118. (b) E. Orgiu, P. Samorì, *Adv. Mater.* 2014, **26,** 1827-1845.

[2] For modulating charge injection at metal-organic interface with a chemisorbed photochromic SAM see: (a) N. Crivillers, E. Orgiu, F. Reinders, M. Mayor, P. Samorì, *Adv. Mater.* 2011, **23**, 1447-1452. (b) T. Mosciatti, M.G. del Rosso, M. Herder, J. Frisch, N. Koch, S. Hecht, E. Orgiu, P. Samorì, *Adv. Mater.* 2016, **28**, 6606.

[3] For hybrid structure combining organic semiconductors blended with Au nanoparticles coated with a photochromic SAM see: C. Raimondo, N. Crivillers, F. Reinders, F. Sander, M. Mayor, P. Samorì, *Proc. Natl. Acad. Sci. U.S.A.* 2012, **109**, 12375-12380.

[4] For blends energy level phototuning in a photochromic - organic semiconductor blend see: (a) E. Orgiu, N. Crivillers, M. Herder, L. Grubert, M. Pätzel, J. Frisch, E. Pavlica, G. Bratina, N. Koch, S. Hecht, and P. Samorì, *Nat. Chem.* 2012, **4**, 675-679. (b) M. El Gemayel, K. Börjesson, M. Herder, D.T. Duong, J.A. Hutchison, C. Ruzié, G. Schweicher, A. Salleo, Y. Geerts, S. Hecht, E. Orgiu, P. Samorì, *Nat. Commun.* 2015, **6**, 6330.

[5] For the fabrication of memory devices: T. Leydecker, M. Herder, E. Pavlica, G. Bratina, S. Hecht, E. Orgiu, P. Samorì, *Nat. Nanotech.* 2016, **11**, 769–775.

[6] For the novel nanomesh scaffold based photodetector: (a) L. Zhang, X. Zhong, E. Pavlica, S. Li, A. Klekachev, G. Bratina, T.W. Ebbesen, E. Orgiu, P. Samorì, *Nat. Nanotech.* 2016, **11**, 900–906. (b) L. Zhang, N. Pasthukova, Y. Yao, X. Zhong, E. Pavlica, G. Bratina, E. Orgiu, P. Samorì, *Adv. Mater.* 2018, **30**, 1801181.

[7] For optically switchable light-emitting transistors: L. Hou, X. Zhang, G. F. Cotella, G. Carnicella, M. Herder, B. M. Schmidt, M. Pätzel, S. Hecht, F. Cacialli, P. Samorì, *Nat. Nanotechnol., 2*019, **14**, 347–353.

[8] For multiresponsive nonvolatile memories based on optically switchable ferroelectric organic FETs: M. Carroli, A. G. Dixon, M. Herder, E. Pavlica, S. Hecht, G. Bratina, E. Orgiu, P. Samorì, *Adv. Mater.*, 2021, **33**, 2007965

Organic Solar Cells – On the Generation and Fate of Free Carriers

D. Neher[1]*

[1] Institute for Physics and Astronomy, University of Potsdam
*e-mail: neher@uni-potsdam.de

Organic solar cells (OSCs) stand out because of their easy processability, flexibility, light weight and the abundance of materials that can act as electron donor (D) or acceptor (A) in the active layer of such devices. Great effort has been put into the development of even a large library of materials, and the appearance of new non-fullerene acceptors (NFAs) has injected new life into the technology, with highest reported efficiencies above 18 %[1]. This is despite the low dielectric constant of organic semiconductors, being the main reason for the exciton nature of the primary excited state and the strong binding of electron-hole pairs through their mutual potential. As such, free charge generation should be strongly field- and temperature dependent while their recombination should proceed at high pace.

The goal of this tutorial is to present techniques and models to analyse and understand the fate of free charges in organic solar cells. We will first address fullerene-based systems with defined energetics and morphology[2,3] before moving on to novel NFA-based systems[4,5]. Barrier-less free charge generation and strongly-suppressed recombination is shown to explain the excellence photovoltaic properties of these devices. We finally discuss how inefficient charge extraction and energetic disorder limits the performance[6] and what is needed to push the device performance towards 20 %.

---

[1] Li, C. et al, *Nat. Energy* 2021, **6** (6), 605–613.

[2] Kurpiers, J.; Ferron, T.; Roland, S.; Jakoby, M.; Thiede, T.; Jaiser, F.; Albrecht, S.; Janietz, S.; Collins, B. A.; Howard, I. A.; Neher, D. *Nat. Commun*. 2018, **9** (1), 2038.

[3] Collado-Fregoso, E.; Pugliese, S. N.; Wojcik, M.; Benduhn, J.; Bar-Or, E.; Perdigón Toro, L.; Hörmann, U.; Spoltore, D.; Vandewal, K.; Hodgkiss, J. M.; Neher, D. *J. Am. Chem. Soc.* 2019, **141** (6), 2329–2341.

[4] Perdigón-Toro, L.; Zhang, H.; Markina, A.; Yuan, J.; Hosseini, S. M.; Wolff, C. M.; Zuo, G.; Stolterfoht, M.; Zou, Y.; Gao, F.; Andrienko, D.; Shoaee, S.; Neher, D. *Adv. Mater.* 2020, **32** (9), 1906763.

[5] Perdigón-Toro, L.; Phuong, L. Q.; Zeiske, S.; Vandewal, K.; Armin, A.; Shoaee, S.; Neher, D. *ACS Energy Lett.* 2021, **6** (2), 557–564.

[6] Tokmoldin, N.; Vollbrecht, J.; Hosseini, S. M.; Sun, B.; Perdigón-Toro, L.; Woo, H. Y.; Zou, Y.; Neher, D.; Shoaee, S. *Adv. Energy Mater.* 2021, **2100804**.

Invited lectures

Lanthanide Complexes as OLED Emission Layers

V.V. Utochnikova[1*]

[1]Lomonosov Moscow State University, Department of Chemistry
*e-mail: valentina.utochnikova@gmail.com

Organic light-emitting diodes (OLEDs) are already a successful commercial product, which is significantly accelerating development in this area. At the same time, there are still a number of unsolved scientific problems in this area, including the development of new technologies and the creation of new materials - potential OLED emitters.

Among them lanthanide coordination compounds (Ln CCs) are still considered as just another class - a minor one due to rather low characteristics: the brightness of OLEDs based on Ln CC of lanthanides rarely exceeds ~10^2 cd/m^2, while for other classes of emitters typical values reach ~10^3-10^4 cd/m^2. However, Ln CCs are fundamentally different from other classes of luminescent compounds. This leads both to the unique possibilities that their use opens up, which are unattainable when using other classes of materials (i.e. incomparably narrow bands with constant position), but also to the need to make significant changes in the process of creating OLED in order to optimize it specifically for this class of compounds.

Based on the data obtained in our group, the features of lanthanide complexes as emitters for OLEDs will be summarized, including those determining their potential role in this area. The reasons for their lower efficiency of electroluminescence in comparison with other classes of emitters will be revealed. The exceptional behavior of the ytterbium ion, emitting in the near infrared region, which surpasses compounds of other classes in the intensity of electroluminescence, will be explained.

This work was supported by RSF (project № 20-73-10053).

Theoretical Prediction of Charge Mobility in Molecular Organic Semconductors

A.Ya. Freidzon[1*]

[1]Federal Research Center "Crystallography and Photonics" Photochemistry Center, Russian Academy of Science

[2] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

*e-mail: freidzon.sanya@gmail.com

Molecular organic semiconductors frequently exhibit hopping charge transport, in which the charge is localized on a certain part of a molecule, the charge mobility is in general lower than in the band-like transport, and the mobility increases with temperature. The unit process of charge hopping is frequently described by the Marcus model. This process can be considered as an electron exchange between two molecules, a neutral one and a radical ion (radical anion for electron transport and radical cation for hole transport). The rate constant for electron exchange of this kind is expressed as follows:

$$k_{et} = \frac{2\pi}{\hbar}|V|^2 \frac{1}{\sqrt{4\pi\lambda k_b T}} \exp\left(-\frac{(\lambda + \Delta G^0)^2}{4\lambda k_b T}\right),$$

where k_{et} is the electron transfer rate constant; k_{b} is Boltzmann constant, T is absolute temperature; ΔG^0 is the Gibbs free energy for the electron or hole transfer reaction; λ is the reorganization energy of the molecule for electron attachment or detachment; and $|V|$ is the so-called hopping integral. All these parameters (ΔG^0, λ, and $|V|$) depend on the molecular structure, conformation, and packing in the layer of an organic semiconductor and can be calculated *ab initio*. One-dimensional charge mobility μ in a direction corresponding to the given dimer can be roughly estimated using the formula

$$\mu \approx \frac{qa^2}{k_b T} k_{et},$$

where k_{et} is the hopping rate constant for the corresponding dimer, q is the electron charge (equal to 1), and a is the hopping distance, taken as a center-to-center distance between monomers in the dimer providing equidistant lattice spacing.

We present an accurate computational technique based on multireference quantum chemistry for predicting k_{et} and μ for different directions in molecular semiconductor crystals. We demonstrate the validity of our procedure with the examples of several hole- and electron-conducting materials.[1, 2]

This work was supported by the Russian Science Foundation (project no. 19-13-00383).

---

[1] Krysko, I.D.; Freidzon, A.Y.; Bagaturyants, A.A. Hole hopping in dimers of N,N′ di(1-naphthyl)-N,N′-diphenyl-4,4′-diamine (α-NPD): a theoretical study. *Phys. Chem. Chem. Phys*., 2020, **22**, 3539–3544.

[2] Freidzon, A.Ya.; Bagaturyants, A.A.; Burdakov, Ya.V.; Nikitenko, V.R.; Postnikov, V.A. Anisotropic Hole Transport in a p-Quaterphenyl Molecular Crystal: Theory and Simulation. *J. Phys. Chem. C*, accepted.

I-3

Balancing the Efficiency, Stability, and Cost Potential for Organic Solar Cells via a New Figure of Merit

J. Min [1*]

[1] The Institute for Advanced Studies, Wuhan University
*e-mail: min.jie@whu.edu.cn

Becuase of the vigorous design and development of organic photovoltaic materials, power conversion efficiency (PCE) is improved rapidly, approaching the threshold of 20%. However, the high costs and intrinsic operational insability of organic solar cells (OSCs) have slowed down its commercialization. In this work, we found that the thermal stability is greatly enhanced as thinner the thickness of active layer. Extended research found that the active layer thickness influences operational stability almost identically as thermal stability for the investigated systems. Thus, a new i-FoM model (i.e., i-FoM2.0)isintroducedasa rational guideline for verifying the true potential of next-generation organic photovoltaic materials in real-world outdoor applications. This work provides a generally available strategy to minimize the efficiency-stability-cost gap and promised the economic prospects of OSCs.

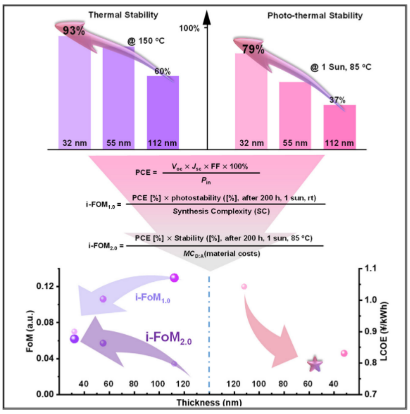


Figure 1: Revlevant figure of merit formulations for evaluating orgnaic photovoltaic materials.

---

[1] Yang, W.; Min, J., et al. *Joule* 2021, **5**(5), 1209-1230.
[2] Min, J., et al. *Adv. Energy Mater.* 2017, **7**(18), 1700465.

I-1

Luminescence Spectroscopy and Microscopy for Conjugated Polymers

I.G. Scheblykin[1*]

Chemical Physics, Lund University
*e-mail: ivan.scheblykin@chemphys.lu.se

In this lecture I will show how we can use luminescence of conjugated polymers to learn about their organization and electronic processes from the level of single molecules to solutions and films. The toolbox which I will use is based on combination of fluorescence microscopy equipped with different types of laser excitation sources and luminescence detection scheme and steady state and time-resolved fluorescence spectroscopy.

If the time allows the following topics will be discussed:

1. How chain conformation and packing influence luminescence spectra and luminescence yield - transition from isolated chains to films.[1]

2. How luminescence polarization can resolve internal organization and energy transfer in conjugated polymers with the help of 2-dimentional polarization imaging technique.[2,3,4,5]

3. How luminescence and light scattering signatures allow to monitor real-time drying of polymer donor/acceptor blends during blade coating deposition.[6]

---

[1] Mirzov, O. & Scheblykin, I. G. G. *Phys. Chem. Chem. Phys.* 2006, **8**, 5569–76.

[2] Camacho, R., Thomsson, D., Yadav, D. & Scheblykin, I. G. *Chem. Phys.* 2012, **406**, 30–40.

[3] Camacho, R., Täuber, D. & Scheblykin, I. G. *Adv. Mater.* 2019, **31**, 1805671.

[4] Shi, J. *et al. Chem. Mater.* 2019, **31**, 8927–8936.

[5] Täuber, D., Cai, W., Inganäs, O. & Scheblykin, I. G. *ACS Omega* 2017, **2**, 32–40.

[6] Liu Y., Yangui A., Berg J., Zhang R., Kiligaridis A., Moons E., Gao F., Inganäs O., Scheblykin I.G., Zhang F. *Small Methods* 2021, DOI: 10.1002/smtd.202100585.

Oral talks

O-1

Selectively Fluorinated Furan-Phenylene Co-Oligomers for Light-Emitting Transistors

I.P. Koskin[1], *C.S. Becker*[1], *A.A. Sonina*[1], *V.A. Trukhanov*[2], *N.A. Shumilov*[1], *A.D. Kuimov*[1],
I.K. Shundrina[1], *D.Yu. Paraschuk*[2], *M.S. Kazantsev*[1]*

[1]N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry SB RAS
[2]Institute of Synthetic Polymer Materials RAS
*e-mail: maximkazantsev1988@gmail.com

Linear conjugated co-oligomers are strongly demanded for organic optoelectronics owing to their inherent lucky combination of high charge carrier mobility and efficient luminescence. Particularly, furan-phenylene co-oligomers (FPCOs) are distinguished by high solubility, molecular rigidity, bright photoluminescence and good hole-transport. However, furan-containing organic semiconductors generally lack electron transport, complicating the realization of efficient furan-based ambipolar light-emitting transistors (OLETs).

Here we report a strategy for improving the optoelectronic performance of FPCOs by selective fluorination. We synthesized 1,4-bis(5-phenylfuran-2-yl)benzene (FP5) derivatives with fully/partially fluorinated central and edge phenyl rings (Fig. 1a). We show that the selective fluorination of FPCOs lowers the energies of frontier molecular orbitals (Fig. 1b), maintaining the bandgap, solubility, bright luminescence, dramatically improves the photostability (Fig. 1c), tunes the π-π stacking, and allows the first realization of electron transport in FPCOs (Fig. 1e).

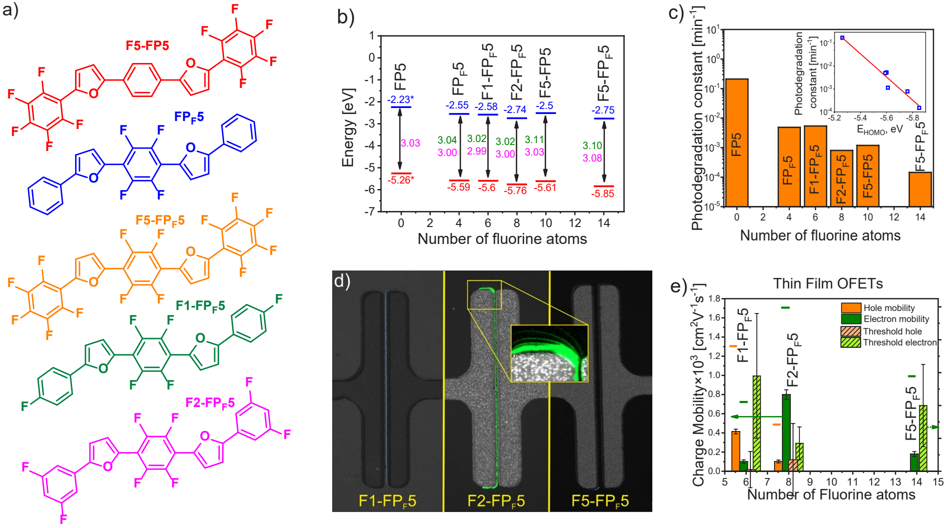


Fig. 1. Chemical structures (a), HOMO/LUMO energies (b), photodegradation constants (c), OLETs (d) and charge mobilities in thin film OFETs of fluorinated FPCOs.

Selectively fluorinated 2,2'-(2,3,5,6-tetrafluoro-1,4-phenylene)bis[5-(3,5-difluorophenyl)furan] demonstrated the best structure, molecular, optoelectronic properties, well balanced ambipolar charge transport and efficient electroluminescence in OLET (Fig. 1d) with external quantum and luminous efficiencies of 0.63% and 5 cdA^{-1}, respectively, which are among the best reported for OLETs. “Smart” selective fluorination is highlighted as a powerful approach to fine-tune the stability and performance of linearly conjugated small molecules for organic optoelectronics.

This work was supported by RSF (project № 20-73-10090).

O-2

Furan-Phenylene Co-Oligomers: Theoretical Modelling Paves Way for the Molecular Smart-Design

I.P. Koskin[1], A.A. Sonina[1], A.D. Kuimov[1], M.S. Kazantsev[1]*

[1]Novosibirsk Institute of Organic Chemistry
*e-mail: osingran@yandex.ru

Linear π-conjugated molecules that exhibit a combination of efficient luminescence and charge mobility attract ever-growing attention due to their possible applications as active materials for organic light-emitting diodes, transistors and lasers. Among all prospective candidates, furan-phenylenes stand out as compounds that are not only effective luminophores and semiconductors but also highly soluble and biodegradable. In the present work, an extensive theoretical study for various furan-phenylene derivatives was carried out to understand underlying structure-properties relationships.

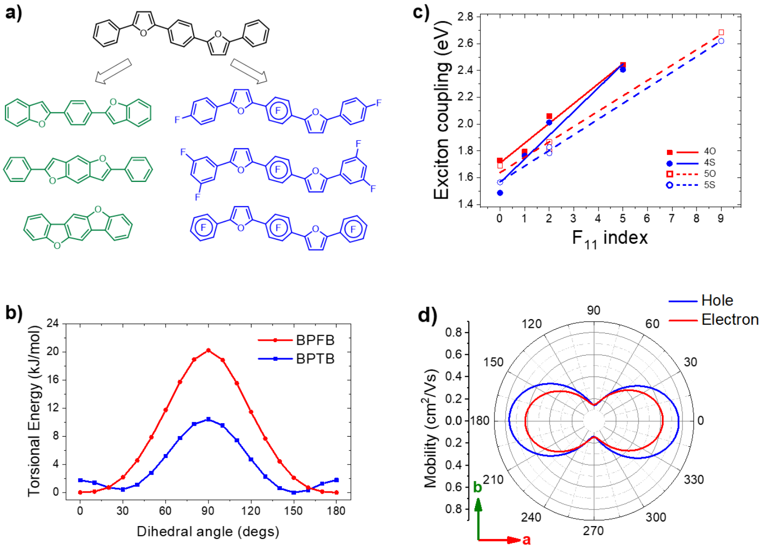


Figure 1. (a) Molecular structure of FP5 and some of the studied annulated and selectively fluorinated derivatives; (b) torsional rigidity of FP5 compared to its thiophene analogue; (c) correlation between annulation index and exciton coupling; (d) calculated angular dependence of charge mobility fluorinated FP5.

Unsubstituted furan-phenylenes (FP5) exhibit high torsional rigidity that facilitates charge transport *via* lowering reorganization energy and increases photoluminescence efficiency by impeding possible quenching pathways. Theoretical study of annulated furan-phenylenes allowed us to derive a quantitative annulation index that accurately predicts molecular properties of annulated compounds without time-consuming theoretical calculations. Fluorinated furan-phenylenes showed greater stability as well as much more effective charge mobility both for holes and electrons. While excessive fluorination of FP5 leads to decreased torsional rigidity, careful and selective fluorination allows achieving the perfect balance between charge mobility, stability and rigidity. All the result, theoretical modeling opens new pathways for molecular smart-design of π-conjugated furan-based semiconductors owing to a deeper understanding of their structure-property relationships.

This work was supported by RSF (project № 20-73-10090).

Methods for Reducing the Lifetime of the Excited State to Increase the Efficiency of Lanthanide-Based OLEDs

M.I. Kozlov[1*], *A.A. Vashchenko*[2], *V.V. Utochnikova*[3]

[1]Lomonosov Moscow State University, Department of Materials Science
[2]Lebedev Physical Institute of the Russian Academy of Sciences
[3]Lomonosov Moscow State University, Department of Chemistry
*e-mail: makariy.kozlov@gmail.com

Lanthanide coordination compounds are promising materials for emission layers of organic light-emitting diodes (OLED), since they have narrow emission bands (up to 10 nm), which will allow achieving high colour purity. However, in contrast to other classes of emitters, which brightness of electroluminescence reaches ~ 10000 cd/m^2, the lanthanide coordination compounds rarely emit an EL brightness higher than ~ 1000 cd/m^2.[1] Thus, obtaining highly efficient lanthanide-based OLEDs is still an urgent and unsolved problem in the development of OLED technology.

One of the main factors limiting the maximum characteristics of lanthanide complexes in OLEDs is the lifetime of the excited state; it is usually ~ 1 millisecond for lanthanide coordination compounds, which increases the probability of roll-off mechanisms and reduces the frequency of radiative recombination of electron-hole pairs. To eliminate the limitation, we proposed several ways to reduce the lifetime: 1) design of lanthanide complexes with readily polarizable ligands and ligands that quench luminescence, 2) synthesis of mixed-ligand complexes, 3) introduction of ytterbium ion into the complex, and 4) use of plasmon resonance.

Hence, as objects of study β-diketonates were chosen as polarizable ligands, and dipyrido [3,2-a:2′,3′-c] phenazine (DPPZ) was used as a neutral ligand, which quenches the luminescence of europium ion. Obtaining the mixed-ligand complexes implies the introduction of different anionic ligands into the composition of one complex, which leads to a decrease in the symmetry of the coordination environment of the central ion, on which the radiation lifetime depends. The effect of an additional ytterbium ion in the composition of europium complexes was also studied: the introduction of ytterbium ion decreases both the quantum yield and the lifetime of the excited state of europium, which can lead to both an increase in the efficiency of the europium electroluminescence and the production of unique organic light-emitting diodes with double emission. The use of plasmon resonance consists in the introduction of gold nanoparticles close to the emission layer, which, according to the literature data, also reduces the lifetime.

The work considers the prospects of the proposed methods for increasing the efficiency of OLED based on mixed-ligand β-diketonates and aromatic carboxylates of europium, terbium, and ytterbium.

---

[1] Kozlov M.I., Aslandukov A.N., Vashchenko A.A., Medvedko A. V., Aleksandrov A.E., Grzibovskis R., Goloveshkin A.S., Lepnev L.S., Tameev A.R., Vembris A., Utochnikova V.V. *Dalt. Trans.* 2019, **48**(46), 17298–17309.

Mesoscopic Modeling of Disordered Morphologies of Blends and Block-Copolymers for Application in Light Emitting Diodes

*J. Zhang[1], K. Kremer[1], J. Michels[1], K.Ch .Daoulas[1]**

[1]Max Planck Institute for Polymer Research
*e-mail: daoulas@mpip-mainz.mpg.de

Recent experiments have demonstrated[1] that the luminous efficiency of polymer light emitting diodes (PLED) can be significantly increased by blending the semiconducting polymer with an insulating homopolymer. Despite the success of this approach, the limited thermodynamic stability of the disordered phase in polymer blends motivates the search for alternative materials. One interesting candidate are block-copolymers (BCPs) comprising semiconducting and insulating blocks.

In this work,[2] we perform computer simulations of disordered blends and their equivalent BCPs of two representative semiconducting and insulating polymers: poly(p-phenylene vinylene) (PPV) and polyacrylate. The simulations are based on a hybrid[3] mesoscopic model, which combines particle- and classical density-functional-based descriptions. Specifically, polymers are coarse-grained into worm-like chains and non-bonded interactions are defined via a quadratic, generic functional of instantaneous local densities of monomers of different chemical species. The functional captures limited compressibility of polymer liquid and repulsion between unlike monomers. The hybrid model serves as a framework for pseudo-dynamical Monte Carlo simulations based on a particle-to-mesh scheme.

We study different compositions and vary immiscibility to mimic annealing at different temperatures. Our simulations demonstrate[2] that disordered blends and BCPs are heterogeneous because of fluctuations and local segregation. We find that local segregation is stronger in BCPs than in their equivalent blends, even though the strength of immiscibility, normalized by the strength corresponding to the mean-field spinodal, is the same. Using a qualitative charge-percolation model, we link the spatial distribution of PPV with electric conductance. We predict[2] that the annealing temperature affects the electrical percolation in disordered BCPs much stronger than in their equivalent blends. The observed differences between blends and BCPs are enhanced at high contents of insulator, which is the regime that is most relevant for practical applications.

---

[1] Abbaszadeh D., Kunz, A., Wetzelaer G. A. H., Michels J. J., Crăciun N. I., Koynov K., Lieberwirth I., Blom P. W. M. *Nature Materials* 2016, **15**, 628-633.

[2] Zhang J., Kremer K., Michels J.J., Daoulas K. Ch. *Macromolecules* 2020, **53**, 523-538.

[3] Daoulas K. Ch., Müller M. *J. Chem. Phys.* 2006, **125**, 184904.

O-5

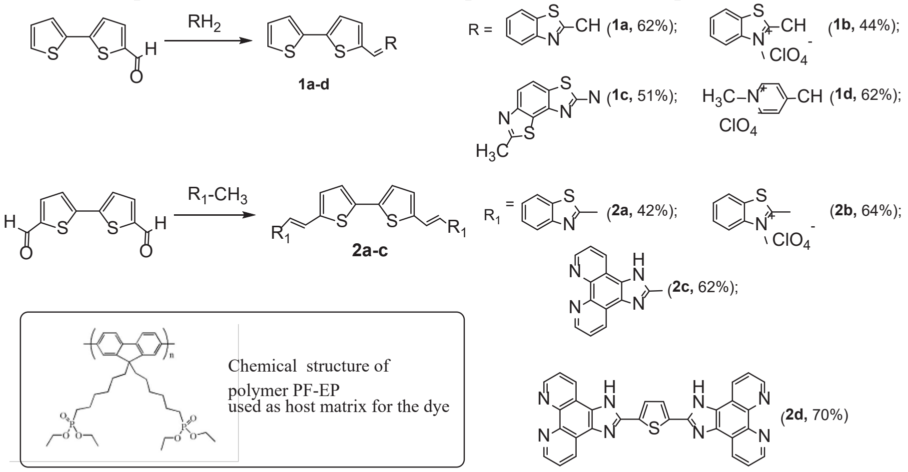
Modification of the Carrier Mobility of Conducting PF-EP Polymer by Doping with Thiophene Derivatives

S.D. Tokarev[1*], *O.A. Fedorova*[1], *Y.V. Fedorov*[1], *D.A. Lypenko*[2], *A.R. Tameev*[2], *E.I. Maltsev*[2]

[1]A.N. Nesmeyanov Institute of Organoelement Compounds RAS
[2]Frumkin Institute of Physical chemistry and Electrochemistry RAS
*e-mail: tokarev@ineos.ac.ru

Conducting polymers have several advantages such as mechanical flexibility, easy processing and transparency which can help in fabrication of cheaper flexible electronic devices. However, their typical charge carrier mobility is very low and need to be improved for efficient devices. Increased attention was directed to study hybrid assemblies based on semiconducting polymers with compounds like non-conducting macromolecules, metals, metal oxides/chalcogenides, and some other inorganic materials. However, the success of these attempts has remained limited. Information on the advantageous use of small molecules as effective dopants in semiconducting polymer composites is still scarce. In our work we synthesized and studied the series of mono- and bithiophene-containing dyes constructed as donor–acceptor π-conjugated systems for doping the polymer matrix. Such molecular structures (D–π–A) are widely investigated as active materials in organic solar cells for they are able to reduce the band gap.

We have found that incorporation of thiophene derivatives (TD) into the PF-EP polymer improves electron transport in the composite. In particular, for composites with TDs **1a**, **1b**, **1c**, **1d**, (5% mass.) the electron mobility increases in the following sequence **1d** < TD free < **1b** < **1a** < **1c**. However, in the operating voltage mode on LEDs with electron transport layers (ETLs) containing these composites, the current and brightness increase in the sequence **1a** < TD free <**1b** < **1d**. This indicates that it is the effective electron injection due to the lower lying LUMO levels of TDs (namely, **1b** and **1d**) relative to the LUMO level in the PF-EP and not electron transport in the ETLs plays a key role in the operation of the manufactured LEDs. The light–emitting diodes made of PF-EP composites containing **1b** and **1d** showed almost two times higher brightness at 15V when compared with a diode made of pure PF-EP. The further synthesis and analysis of such structures may be considered as a promising approach to the development of new electroactive composites with better optoelectronic characteristics.



Chemical structure of polymer PF-EP used as host matrix for the dye

Fig. 1 Structures of dyes **1a-d**, **2a-d**, and polymer host matrix.

This work was supported by RSF (project № 17-73-30036-П).

O-6

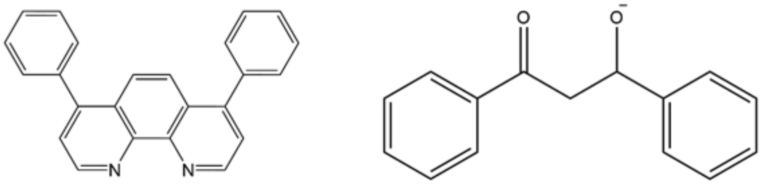
Ytterbium-Europium Dibenzoylmethanates with Bathophenanthroline in OLEDs

A.I. Kornikov[1],M.I. Kozlov[2], V.V. Utochnikova[1]*

[1]Lomonosov Moscow State University, Chemistry Department
[2]Lomonosov Moscow State University, Department of Materials Science
*e-mail: andrey.i.kornikov@gmail.com

Lanthanide coordination compounds are promising materials for emission layers of organic light-emitting diodes (OLEDs), since lanthanide ions, due to their special electronic structure, demonstrate narrow luminescence bands. One of the forward-looking applications of OLED is oximetry, a non-invasive spectrophotometric method of determining the degree of oxygen saturation in the blood. However, a big challenge to OLED technology for oximetry is obtaining OLEDs with luminescence in both visible and near-infrared ranges. The use of bimetallic rather than separate monometallic complexes will allow creating an oximeter, which uses one light-emitting diode instead of two. Even though europium and ytterbium ions have ideal narrow luminescence bands for oximetry, lanthanide-based oximeters have not been obtained yet. Thus, it was proposed to study the luminescent properties of bimetallic complexes of europium and ytterbium, possessing two emission bands in both the red and infrared regions of the spectrum.

Bathophenanthroline (BPhen) (Figure 1), which is capable of sensitizing Eu^{3+} ion luminescence and providing high electron mobility, was chosen as a neutral ligand.[1] The dibenzoylmethanate anion (dbm^-) (Figure 1) was chosen as the anionic ligand (Fig. 1), since its europium complex shows intense luminescence. Thus, the objects of the study are mixed-ligand complexes $Eu_xYb_{1-x}(dbm)_3BPhen$ (x = 0; 0.01; 0.02; 0.03; 0.05; 0.07; 0.1; 1), as well as $Eu_xLa_{1-x}(dbm)_3BPhen$ and $La_xYb_{1-x}(dbm)_3BPhen$ (x = 0; 0.01; 0.02; 0.1). The aim of this work was to obtain an efficient OLED with dual emission of europium and ytterbium.



BPhen **dbm^-**

Figure 1. Structural formulas of the ligands

The composition of the obtained compounds was determined by the thermogravimetric analysis, IR spectroscopy, ^1H NMR spectroscopy, and scanning electron microscopy with EDX. The quantum yields of the ytterbium complexes photoluminescence reached 1.2%, which is rather high, and the individual europium complex demonstrated a quantum yield of 75%. OLED study of the obtained complexes demonstrated that among them $Eu_{0.01}Yb_{0.99}(dbm)_3BPhen$ exhibited dual emission in the visible and near-infrared regions of comparable intensity and the most intense electroluminescence of ytterbium.

---

[1] Kozlov M.I., Aslandukov A.N., Vashchenko A.A., Medvedko A. V., Aleksandrov A.E., Grzibovskis R., Goloveshkin A.S., Lepnev L.S., Tameev A.R., Vembris A., et al. *Dalt. Trans.* 2019, **48**(46), 17298–17309.

Spectroscopic Assessment of Charge-Carrier Mobility in Organic Semiconductors

O.G. Kharlanov[1,2*], D.R. Maslennikov[1,2], E.V. Feldman[1], G.G. Abashev[3], O.V. Borshchev[4], S.A. Ponomarenko[4], M.V. Vener[2,5], D.Yu. Paraschuk[1,2], A.Yu. Sosorev[1,2]

[1]Lomonosov Moscow State University, Department of Physics
[2]Institute of Spectroscopy, RAS
[3]Perm State National Research University, Faculty of Chemistry
[4]Enikolopov Institute of Synthetic Polymeric Materials, RAS
[5]Mendeleev University of Chemical Technology of Russia, Dept. of Quantum Chemistry
*e-mail: kharlanov@physics.msu.ru

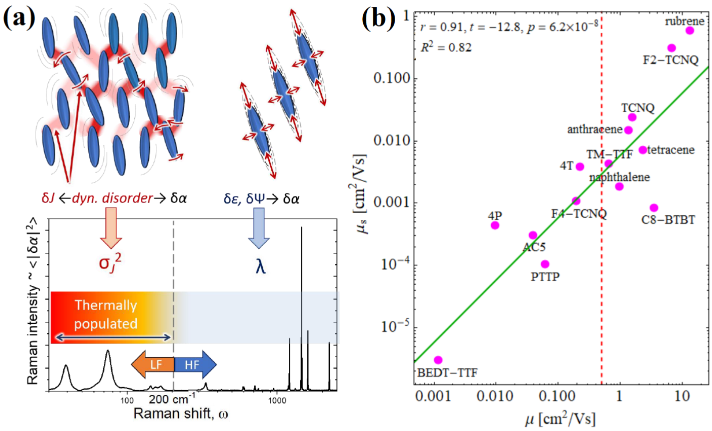


Figure 1. (a) Relationship between low- and high-frequency Raman spectra and electron-phonon interaction in organic semiconductors. (b) Correlation between spectroscopically estimated charge-carrier mobilities μ_s and device mobilities μ in various OS materials.

Further progress in organic electronics demands new highly efficient organic semiconductor materials. So far, however, band-like charge transport with high mobilities has been reliably demonstrated only in a few organic semiconductors (OSs), and development of efficient methods for search of high-mobility materials among a plethora of OSs remains extremely important. We suggest a spectroscopic method for screening of OSs with efficient charge transport, to be used prior to time-consuming device measurements. The method relies upon a physical relationship between the low-frequency Raman spectrum and the non-local electron-phonon interaction and dynamic disorder limiting charge-carrier mobility in OS materials (Figure 1a).[1,2,3] Experimental benchmarking of the physics-inspired spectroscopic descriptor for charge-carrier mobility estimation resulting from this relationship reveals a strong correlation with device mobilities reported for various OSs (Figure 1b). We thus anticipate that the spectroscopic method based on this descriptor can serve as a powerful search tool for revealing new high-mobility OS materials.

The research was supported by the Russian Science Foundation (project № 18-72-10165).

---

[1] Sosorev A.Yu. *et al., Phys. Stat. Sol. – RRL* 2019, **13**, 1800485.

[2] Nuraliev M.K. *et al.,* J. Chem. Phys. *J. Chem. Phys.* 2020, **153**, 174303.

[3] Vener M.V. *et al.*, *Adv. Electron. Mater.* 2021, **7**, 2001281.

O-8

Spiroconjugation Effect on Optoelectronic Properties of Spirobi[indene]-1,1'(3*H*,3'*H*)-diones with Extended Conjugation

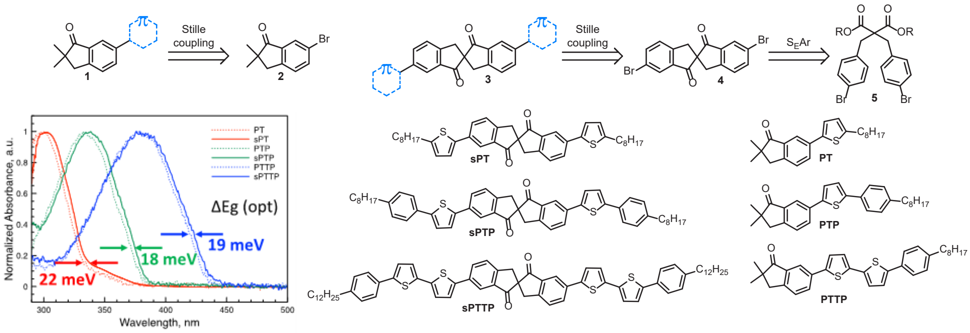
<u>*K.S. Ivanov*</u>*[1]*, T. Riesebeck[1], A.D. Skolyapova[1], I.V. Liakisheva[1], M.S. Kazantsev[1,2], R.Yu. Peshkov[1], K.M. Shepovalov[1], E.A. Mostovich[1]*

[1]Novosibirsk State University
[2]N.N. Vorozhtzov Novosibirsk Institute of Organic Chemistry SB RAS
*e-mail: konstantin.s.ivanov@mail.ru

High-performance organic semiconducting devices such as organic light-emitting diodes (OLEDs) and organic light-emitting transistors (OLETs) require materials combining efficient electroluminescence and high semiconducting properties. However, synthesis of such compounds is a non-trivial task since the dense packing that is crucial for improved semiconducting properties causes quenching of luminescence due to the aggregation effects.

Spiroconjugated aromatic compounds comprise a molecular architecture in which two orthogonal π-systems are forced to homoconjugate with each other through a quaternary spiro carbon center. The extent of spiroconjugation can be adjusted with the substitution pattern around the spiro center. In addition, spiro compounds provide with the possibility of asymmetric modification with donor and acceptor on each side of spiro center. This can open up prospects for various properties like charge-transfer, TADF or singlet fission.

Here we present a scope of synthesis, structure, chemical modifications as well as optical and electrochemical properties of spirobi[indene]dione derivatives as one-dimensional materials.



The absorption and fluorescence were registered for all the compounds. Noteworthy, absorption and emission maxima are red-shifted for the spirocyclic compound **sPT**, **sPTP**, and **sPTTP** in comparison to their parent non-spiro structures **PT**, **PTP**, and **PTTP** respectively. Spiroconjugation effect value was shown to lie in the range of 19-22 meV, which corresponds with cyclovoltammetry data.

Quantum chemical calculations were used for theoretical study of ground and excited states geometries, frontier orbitals electronic densities, singlet and triplet states energy. As a result, it was shown that spiroconjugation could be effectively used for designing materials with precise tuning of specific optical and electronic properties.

This work was supported by Russian Science Foundation (project № 19-13-00327) and Ministry of Science and Higher Education of Russian Federation project No FSUS-2020-0036.

O-9

Density of States in Locally Ordered Amorphous Organic Semiconductors: Emergence of the Exponential Tails

S.V. Novikov[1,2*], *A.R. Tameev*[1,2]

[1]A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS
[2]National Research University Higher School of Economics
*e-mail: novikov@elchem.ac.ru

Density of states (DOS) is one of the most important characteristics affecting charge carrier transport in organic semiconductors. The total shape of the DOS in the particular material is typically rather complicated. Fortunately, for the consideration of the charge transport properties at typical operating temperatures the deep tail of the DOS is most important, and the problem becomes much more tractable. Two popular models of the tail are the Gaussian model and exponential model. Here we consider a new mechanism of the formation of the exponential tails in locally ordered amorphous organic semiconductors.[1] The starting point is the model of the qudrupolar glass having the DOS dominated by electrostatic contributions, which is suitable for the description of many nonpolar organic materials. We assume that the quadrupoles are arranged in blocks and the orientations of all quadrupoles in the block is the same while the orientations in different blocks are random. It turns out that for blocks having linear size of about 5 molecules or more the tails become exponential, while for the totally random orientation of all quadrupoles they have the Gaussian shape (Figure 1).

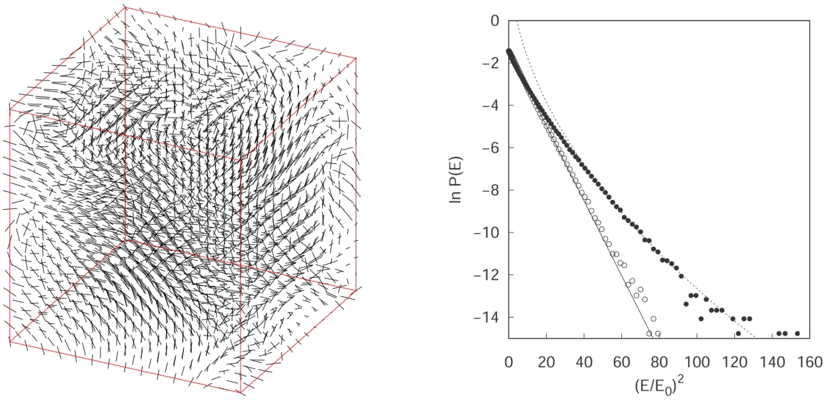


Figure 1. Typical spatial distribution of axial quadrupoles (left) and the DOS for the average linear size of the block equals to 5 molecules (right, empty circles show the low energy tail and the filled circles show the high energy tail, broken line shows the best exponential fit, solid line corresponds to the Gaussian central peak). Parameter $E_0 = eQ/\varepsilon a^3$ is the scale of energy (here Q is the quadrupole moment, a is the lattice scale, and ε is the dielectric constant). We assume that $eQ > 0$, for the opposite sign of eQ the tails are interchanged.

For the quadrupoles having axial symmetry the DOS is asymmetric, while for planar quadrupoles it is symmetric. Particular structure of the blocks is not very important and the only significant parameter is the average size of the blocks (their shape could be random or regular, e.g. cubic, interfaces between blocks could be sharp or smoothed). For this reason we believe that the suggested mechanism of the formation of the exponential tails is rather common and may occur in various organic materials.

This work was supported by RFBR (project № 18-29-23045 mk).

---

[1] S.V. Novikov, *J. Chem. Phys.* 2021, **154**(12), 124711.

O-10

Off-Diagonal Disorder and Field-Assisted Diffusion in Disordered Organic Semiconductors

M.D. Khan[1], *V.R. Nikitenko*[1]*

[1]National Research Nuclear University “MEPhI” (Moscow Engineering Physics Institute)
*e-mail: vladronik@yandex.ru

One of the main analytical tools for the modelling of charge transport is the multiple trapping and release (MTR) model[1] in the framework of the Gaussian disorder model (GDM).[2] In this work, we generalized the MTR approach[1] in such a way that each deep hopping state is described in addition to its energy E by an additional parameter that characterizes the random spatial environment of an individual center. One can approximate the distribution of this parameter by a Gaussian function with the width Σ. Being temperature-dependent, it differs from the non-diagonal disorder parameter Σ_B of the GDM. In the sense of GDM, we consider the maximal possible non-diagonal disorder. Our model gives the same values and temperature dependence of the quasi-equilibrium mobility as the conventional GDM-MTR approach[1,2], but taking into account the additional scatter in the release rates of a carrier from deep states gives a significant increase in the field-assisted diffusion coefficient. It results in anomalously wide transient current tails in time-of-flight (TOF) experiments.[3]

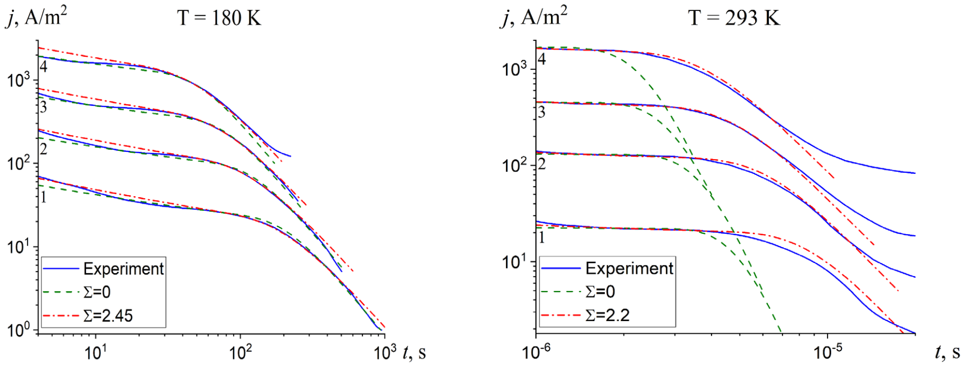


Figure 1 Comparison of calculation results with experimental TOF data[3]. L=3,6 µm. Applied voltage, V: 1- 150, 2- 190, 3- 230, 4- 270.

Our model gives good description of TOF transient currents[3] in a wide range of temperatures and field strengths, $F=V/L$, while calculations with purely energy disorder cannot describe the TOF transients at different temperatures, see the dashed curves in Figure 1. The anomalous dispersion of transient currents must be taken into account for the correct determination of the mobility and width of the Gaussian energy distribution from the TOF data;[2] therefore, a correct description of field-assisted diffusion is necessary for a complete and correct analysis of the TOF data.

This work was supported by the Russian Foundation for Basic Research (RFBR), project number 19-32-90088.

---

[1] Khan M.D., Nikitenko V.R., Tyutnev A.P., and Renat Sh. Ikhsanov R.Sh., *J. Phys. Chem. C* 2019 **123**, 1653−1659.

[2] Bässler H., *Phys. Stat. Sol. B* 1993 **175**, 15-56.

[3] Mozer A.J., Sariciftci N.S., Pivrikas A., Österbacka R., Juška G., Brassat L., and Bässler H., *Phys. Rev. B* 2005 **71**, 035214.

O-11

DFT Benchmark of Geometry and Excited States of Spiro[4,4]nona-1,3,6,8-tetraene

R.Yu. Peshkov[1*], *K.M. Shepovalov*[1], *E. Benassi, E.A. Mostovich*[1]
[1]Novosibirsk State University, Laboratory of Organic Electronics
*e-mail: r.peshkov@nsu.ru

Spiroconjugated molecules, i.e. containing two orthogonal weakly interacting π-systems, attract great attention for optoelectronic applications due to their high intrinsic rigidity, small reorganization energy, versatile optical, electronic and morphology properties[1]. Spiro-compounds were demonstrated to be excellent hole transporting materials, efficient intramolecular through-space charge-transport leading to TADF[2] and more[3]. Among the variety of 2D- and 3D-spiroconjugated materials, 1D-materials are still uncovered, mainly due to synthetic challenges. Spiro[4,4]nona-1,3,6,8-tetraene, the central rigid core for π-extended 1D-spirosystems, synthesized in 1970th, though was studied with semi-empirical and early DFT methods[4], had never been an object of detailed ground/excited states studies within modern DFT. We describe DFT benchmark to select the most suitable method for prediction of desired optoelectronic properties of novel spiroconjugated materials. Among number of pure and hybrid DFT functionals and Hartree-Fock method, coupled with three basis sets, HF found as the best for ground state geometry optimization and frequency analysis. Prediction of excited states energies within TD-DFT and Tamm-Dancoff approximation demonstrated that long-range corrected functionals CAM-B3LYP and ωB97XD, together with M06-2X, are more productive for singlet states calculations, B3LYP and PBE0 – for triplets. Selected method can be used for optoelectronic properties prediction and design of novel one-dimensional spiroconjugated materials with extended conjugated systems.

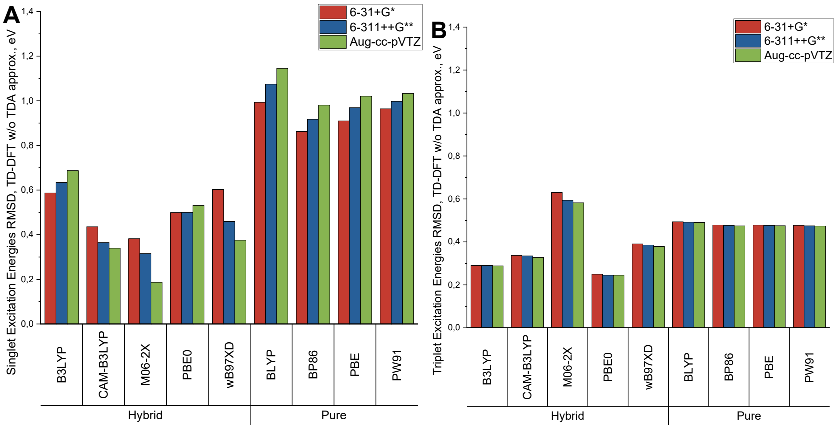


Fig. 1. Benchmark results of excited states energies prediction

This work was supported by RSF (project № 19-13-00327) and Ministry of Science and Higher Education (project № FSUS-2020-0036).

---

[1] Saragi T. P. I., Spehr T., Siebert A., Fuhrmann-Lieker T., Salbeck J. *Chem. Rev.* 2007, **107** (4), 1011–1065.

[2] Yang S., Wang Y., Peng C., Wu Z., Yuan S., Yu Y., Li H., Wang T., Li H., Zheng Y., Jiang Z. and Liao L. *J. Am. Chem. Soc.* 2020**, 142**(41), 17756–17765.

[3] Liu S., Xia D. and Baumbarten M. *ChemPlusChem* 2020, **86**(1), 36–48.

[4] Haselbach E., Allan M., Bally T., Bednarek P., Sergenton A., de Meijere A., Kozhushkov S., Piacenza M. And Grimme S. *Helvetica Chimica Acta* 2001, **84**(6), 1670–1693.

Role of the Reorganization Energy for Charge Transport in Disordered Semiconductors

R. Saxena[1*], *V.R. Nikitenko*[2], *I.I. Fishchuk*[3,4], *Ya.V. Burdakov*[2], *Yu.V. Metel*[2], *J. Genoe*[5], *H. Bässler*[6], *A. Köhler*,[1,6] *A. Kadashchuk*[4,5]

[1] Soft Matter Optoelectronics and Bavarian Polymer Institute (BPS), University of Bayreuth
[2] National Research Nuclear University "MEPhI" (Moscow Engineering Physics Institute)
[3] Institute for Nuclear Research, National Academy of Sci. of Ukraine
[4] Institute of Physics, National Academy of Sciences of Ukraine
[5] Interuniversity Microelectronics Centre (IMEC)
[6] Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth
*e-mail: rishabh.saxena@uni-bayreuth.de

While it is commonly accepted that the activation energy of the thermally activated polaron hopping transport in disordered organic semiconductors can be decoupled into a disorder and a polaron contribution, their relative weight is still controversial. This feature is quantified in terms of the so-called C-factor in the expression for the effective polaron mobility: $\mu_e \propto exp[-E_a/k_BT - C(\sigma/k_BT)^2]$, where E_a and σ are the polaron activation energy and the energy width of a Gaussian density-of-states (DOS), respectively. A key issue is whether the universal scaling relation (implying a constant C-factor) regarding the polaron formation energy is really obeyed in the same disordered system, as recently claimed in literature.[1] In the present work, we reinvestigate this issue on the basis of the Marcus transition rate model using extensive kinetic Monte Carlo simulations as a benchmark tool. We compare the polaron-transport simulation data with results of analytical calculations by the effective medium approximation (EMA) and multiple trapping and release (MTR) approaches. The key result of this study is that the C-factor for Marcus polaron hopping depends on first whether quasiequilibrium has indeed been reached, further on the σ/E_a ratio (Figure 1a), and finally on the degree of carrier localization, i.e., the coupling between the sites (Figure 1b). This implies that there is no universal scaling with respect to the relative contribution of polaron and disorder effect. Finally, we demonstrate that virtually the same values of the disorder parameter σ are determined from available experimental data using the C-factors obtained irrespective to whether the data are interpreted in terms of Marcus or Miller-Abrahams rates. This implies that molecular reorganization contributes only weakly to charge transport, and it justifies the use of the zero-order Miller-Abrahams rate model for evaluating the DOS width from temperature dependent charge transport measurements.

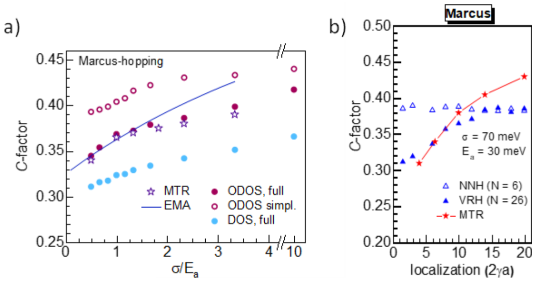


Figure 1. C-factor vs. a) σ/E_a ratio ($2\gamma a = 10$) and b) localization parameter derived using Marcus rate in an isotropic 3D system. "DOS, full" refers to the case of non-equilibrated transport, all other data is obtained for transport under equilibrium.

---

[1] K. Seki and M. Wojcik, *J. Chem. Phys.* 2016, **145**, 034106.

The Mechanism of Changing the Organic Field-Effect Transistors (OFETs) Electrical Properties Under Toxic Gases Exposure

D.S. Anisimov[1], *A.A. Trul*[1], *V.P. Chekusova*[1], *A.A. Abramov*[1], *E.V. Agina*[1], *S.A. Ponomarenko*[1]

[1]Enikolopov Institute of Synthetic Polymeric Materials, Russian Academy of Sciences
*e-mail: anisimov@ispm.ru

Thin-film organic field-effect transistors (TF-OFETs) are extremely promising as gas sensors due to their outstanding sensitivity and low production cost provided by scalable solution processing. The sorption of polar gases to the active layer affects the electrical properties of the devices. Monomolecular films can increase the sensitivity and decrease the response time, which is actively used for various gases detection.[1] At the same time, there is still no theoretical model describing the sensory properties in connection with the electrical characteristics of individual OFETs, such as operating currents, charge carrier mobility, and threshold voltage or kinetic parameters associated with their degradation over the time. The literature data show only a few correlations of the OFETs electrical properties with their sensory sensitivity, which are valid for strictly defined materials and device architectures[2] and cannot describe more general cases.

In this work, we aim to reveal the correlation of the electrical characteristics of a field effect transistor, such as carrier mobility, threshold voltage, subthreshold slope, transfer curve hysteresis, and bias stress characteristic time with sensory properties of the gas sensors based on them, such as detection limit and sensitivity. Since it is well known that there are charge traps in the transistor channel, which determine both the electrical and sensory properties of the OFET,[3] therefore, we analyze each of these parameters in connection with the density of the trap states in order to develop an operation model of the OFET-based sensors.

We analyze field-effect transistors based on thin vacuum evaporated films of the C8-BTBT-C8 semiconductor on the top of various dielectrics intrinsically having different densities of surface charge traps and further modulate it with additional treatment via UV-irradiation, which can controllably create additional traps. We have fully characterized electrical properties of sensors and their response to nitrogen dioxide and examined the sensitivity correlations with individual electrical parameters. It was shown that trap density derived from bias stress kinetic and threshold voltage shows the highest correlation with sensitivity which is consistent with the key role of deep charge traps in gas detection mechanism. This work takes the first steps towards predicting of OFETs sensory properties on the base of their electrical properties which can be measured much faster and paves the way to propose a novel model of OFET-based gas sensors sensitivity.

This work was supported by the Russian Foundation for Basic Research project №20-03-00810.

---

[1] Sizov A., et al., *ACS applied materials & interfaces*, 2018, **10**(50), 43831–43841

[2] Duarte D., et al., *Journal of Applied Physics*, 2012. **111**(4): p. 044509.

[3] Huang W., et al., *Advanced Materials*, 2017. **29**(31): p. 1701706.

Self-Assembly of Recyclable Supramolecular 1D Semiconductors from bis-Phthalocyanines on Solid Surfaces

A.I. Zvyagina[1*], *A.E. Aleksandrov*[1], *A.G. Martynov*[1], *A.R. Tameev*[1], *A.E. Baranchikov*[2],
A.A. Ezhov[3], *Yu.G. Gorbunova*[2], *M.A. Kalinina*[1]

[1] A. N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS
[2] N. S. Kurnakov Institute of General and Inorganic Chemistry RAS
[3] Moscow State University, Department of Physics
*e-mail: zvyagina.ai@gmail.com

Fabrication of processable one-dimensional (nano)semiconductors and their arrangement on solids are among major challenges for organic electronics. Supramolecular aggregation of aromatic discotics such as phthalocyanines have gained attention as a strategy for creating tubular nanostructures in a controlled fashion but their electric properties remain relatively low. Herein, we describe cooperative self-assembly of lutetium crown-substituted double-decker phthalocyaninate (LuL_2) via crown-assisted coordination with K^+ for fabricating supramolecular nanowires with an average length up to 50 µm, thickness down to 5 nm. The conductivity of the film obtained with deposition of nanowires from the dispersion in chloroform under slow evaporation of the solvent is 11.4 $S \cdot cm^{-1}$. This value is the highest measured in non-doped phthalocyanine assemblies. The ability of crown-groupes of the LuL_2 complex to interact with K^+ ions dictate the full conjugation of macrocyclic rings of phthalocyanine complexes in 1D aggregate and the efficiency of charge transfer along the nanowires.

The high sensitivity of K^+-LuL_2 assemblies to the electric field makes it possible to use field-assisted method for the arrangement of the already prepared nanowires on solid supports. The voltage applied between the electrodes guides the oriented deposition of the already formed nanowires from their solution onto the surface. The nanowires are oriented along the field lines from anode to cathode immediately after field switch on. The deposition proceeds within 20 minutes yielding the continuously ordered layer of nanowires on the support. The packing density of the nanowires within the layer can be tuned by varying the concentration of K^+-LuL_2 dispersion.

The recyclability of the self-assembled nanowires is a significant advantage over conventional covalently linked polymers for fabricating organic-based devices for a next-generation “green” electronics. The K^+-LuL_2 nanowires, otherwise stable in water and most organic solvents, can be easily disintegrated into starting components in acetonitrile and then separatied for further re-application without adding any other chamicals.

Our results demonstrate the potency of supramolecular strategy based on self-assembly for fabricating semiconductor nanowires with high electric properties from organic molecules with large aromatic system, such as phthalocyanines. Cooperative process involving weak intermolecular oordination bonds provide full conjugation of electronic systems of phthalocyanines for efficient charge transfer along nanowires. Although the cooperative binding provides stability to the as-formed structures, the bond weakness makes it possible to desintegrate these nanowires in a good aprotic solvent for further recycling.

This work was supported by Russian Science Foundation (№19-73-00025).

Liquid Luminophores Based on Organic π-conjugated Oligomers with Alkylsilyl Solubilizing Groups

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

[1]Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Sciences
*e-mail: luponosov@ispm.ru

The liquid organic luminophores (LOL) have several intriguing properties and can find application in organic electronics and photonics.[1] They do not require using and then removing solvents at the processing. The LOL can act as a solvent with a high quantum yield of luminescence for other luminescent organic and hybrid dopants. Nowadays, LOL are intensively developed and studied. However, existing variety of LOL is presented by families of compounds emitting light mainly in a short-wave part of UV-Vis spectrum. However, luminophores emitting light in long-wave region (yellow – red) usually consist of a larger number of conjugated blocks and may contain strong electron-withdrawing fragments. Therefore, a molecular design of such LOL is not trivial and requires using very effective solubilizing groups (SG). In this work, the synthesis of oligomers having a rigid conjugated 4,4'-bis(2-thienyl)biphenyl fragment end-capped with various types of solubilizing groups (SGs), such as either alkyl or alkylsilyl or alkyloligodimethylsiloxane, has been reported.[2] The comprehensive study of their thermal and optical properties as well as rheology in comparison to model highly crystalline oligomers with simple either hexyl or trimethylsilyl SGs allowed us to elucidate structure–property correlations and find the most powerful type of SG in terms of liquefaction for them. Next, we extended our strategy and prepared a series of similar liquid luminophores having additional either 2,1,3-benzothiadiazole or 5,6-difluoro-2,1,3-benzothiadiazole central units in the structure and as result emitting light in a long-wave part of UV-Vis spectrum.

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

---

[1] F. Lu, T. Nakanishi, *Adv. Optical Mater.* 2019, **1900176**.

[2] Yu.N. Luponosov, D. Balakirev, I. Dyadishchev, A.N. Solodukhin, M.A. Obrezkova, E.A. Svidchenko, N.M. Surin, S. Ponomarenko, *J. Mater. Chem. C*, 2020, **8,** 17074.

Enhancement of Light-Emitting Properties of 2D Organic Semiconductors via Molecular Doping

A.V. Kuevda[1,2*], *R.S. Fedorenko*[2,3], *V.A. Trukhanov*[2,3], *O.V. Borshchev*[2], *D.Yu. Paraschuk*[2,3]
[1]Skolkovo Institute of Science and Technology
[2]Enikolopov Institute of Synthetic Polymeric Materials, Russian Academy of Sciences
[3]Faculty of Physics, Lomonosov Moscow State University
[*]e-mail: alexey.kuevda@skoltech.ru

Organic light-emitting semiconducting devices require materials combining efficient charge transport and bright luminescence. The latter is easily achieved in isolated molecules, while the former can be realized in highly aggregated systems, which usually quench luminescence. This dilemma can be solved by introducing into the host matrix highly luminescent dopant molecules, which accept the excitation energy from the host via exciton diffusion and Forster resonant energy transfer. Such molecular doping approach is well-known for thick (3D) organic semiconductor crystals but not for 2D ones that include one or a few molecular layers. Such 2D films are very promising for organic light-emitting transistors as they are intrinsically free of such drawbacks known for 3D organic light-emitting transistors as light waveguiding and contact effects.[1,2] Here we report on molecular doping in 2D organic semiconductor crystals, which significantly increases light-emitting properties of 2D films.

We chose specific organic semiconducting materials for host matrix and guest dopant,[3] considering their structural resemblance (Fig. 1, right bottom inset) and an overlap of photoluminescence (PL) spectrum of the host with an absorption spectrum of a guest. We found that the doped films PL spectra contain new bands, similar in their positions to ones of the dopant molecules, and these peaks have higher intensity than those of the host (Fig. 1, right top inset). From this data we conclude that host-guest energy transfer operates in the 2D doped films. Then we fabricated organic light-emitting transistors with the doped 2D film as an active layer, which show electroluminescence (Fig. 1, left top inset). The electroluminescence spectrum well corresponded to the PL one (Fig. 1, right top inset).

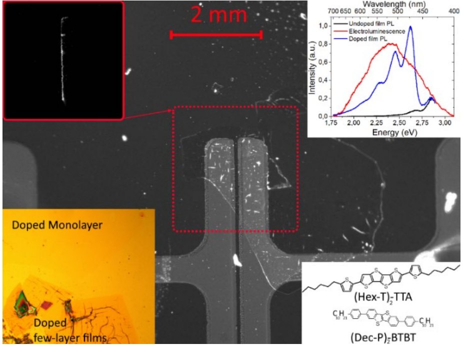


Figure 1. Organic light-emitting transistor with active layer based on solution-processed 2D (Dec-P)$_2$-BTBT film doped with 1% of (Hex-T)$_2$-TTA (bottom left). Electroluminescence recorded is in the top left inset, optical image of the 2D doped film is in the left bottom inset, spectra of PL of the doped, reference undoped film and electroluminescence are in the top right inset.

This work was made with support of RSCF №18-12-00499

---

[1] E. V. Agina, et al. *ACS Appl. Mater. Interfaces* 2017, **9**(21), 18078–18086.
[2] V. V. Bruevich, et al. *ACS Appl. Mater. Interfaces* 2019, **11**(6), 6315-6324.
[3] O. V. Borshchev, et. al. Dyes and Pigments, 2021, **185**, 108911.

O-17

Cascade Reactions in Seven-Membered Systems: Towards Innovative Functional Materials

R.F. Salikov[1*], *Y.V. Tomilov*[1]

[1]N. D. Zelinsky Institute of Organic Chemistry RAS
*e-mail: rinat_salikov@ioc.ac.ru

Cascade reactions have been a potent approach to develop new carbo- and heterocyclic systems. The cascades employing electrocyclic transformations open the way to the synthesis of hepta(methoxycarbonyl)cycloheptatrienyl potassium and penta(methoxycarbonyl)cyclopentadienyl potassium or sodium. Both the syntheses include addition of a common vinylpyridinium intermediate to CH-acids (Fig. 1).[1] The two obtained products were found to be quite universal synthons for the synthesis of promising functional materials. In particular, penta(methoxycarbonyl)cyclopentadienyl anion was used in the synthesis of novel dyes containing the proaromatic hydrazinylidenecyclopentadiene acceptor fragment. Two compounds were tested in bulk heterojunction solar cells. The maximum efficiency achieved so far for the devices under study comprised 2%.[2]

Moreover, electrocyclic transformations of hepta(methoxycarbonyl)cycloheptatrienyl potassium in a reaction with amines gave new fluorescent electron-defficient 5-hydroxyisoquinolones.[3] A large Stokes shift was registered for the synthesized class of fluorescent dyes along with a noticeable quantum yield. Additionally, 5-hydroxyisoquinolones demonstrated superphotoacidic properties, i.e. an increase in acidity in excited state, which holds promises for various applications such as enhancing photo-induced cation polymerization.

Other cascade reactions of vinylpyridinium with CH-acids gave cycloheptadienes. bicycloheptenes or pyridinium cyclopentadienolate which in turn gave a series of donor-acceptor chromofores wherein the presence of additional reaction centers gave rise to futher stepwise modifications that allowed to control compounds' absorption spectra.[4]

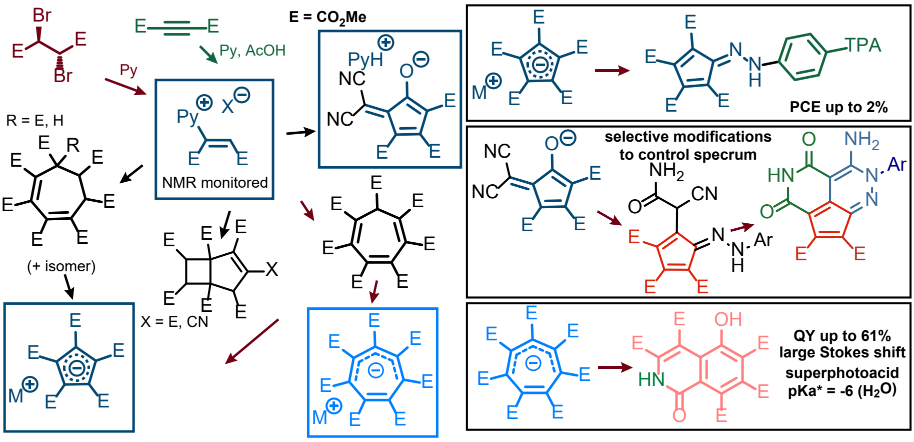


Fig. 1. Synthesis and the use of precursors to functional materials.

This work was supported by RFBR (project № 20-33-70263).

---

[1] *Synlett.* **2018**, 1157; *Eur. J. Org. Chem.* **2018**, 5065.
[2] *Dyes Pigm.* **2019**, 500; *Mend. Commun.* **2019**, 304.
[3] *Dyes Pigm.* **2021**, 109107.
[4] *Dyes Pigm.* **2021**, 109132.

Sponsor talk

Imaging Ellipsometry and Near-Field Microscopy Techniques for Organic Electronics Applications

M.A. Trusov[1*]

[1]IMC Group Ltd.
*e-mail: trusov@imc-systems.ru

Imaging ellipsometry is an all-optical, non-contact metrology technique that excels at the layer-thickness and material characterization of micro-structured thin-film samples and substrates. The technique combines microscope imaging with the measurement principles of spectroscopic ellipsometry. It reaches a spatial resolution of about 1 μm, easily beating the limits of other optical metrology tools such as regular ellipsometers, reflectometers, and polarization-contrast microscopy. Accurion's imaging ellipsometers combine the benefits of ellipsometry and optical microscopy into a single advanced research instrument. The enhanced spatial resolution of imaging ellipsometers expands ellipsometry into new areas of microanalysis, microelectronics, and bio-analytics.

Scanning near-field optical microscopy (SNOM) breaks the diffraction-related limitation for the optical analysis methods. Recent advancements in scattering SNOM developed by NeaSpec team provide high-level tools to perform artifact-free nano-scale optical characterization with wavelengths from VIS and IR to THz with a broad range of applications in various research fields. In our talk we will also introduce the technology of nano-FTIR by NeaSpec, and show some new interesting measurements results.

O-18

Conduction Band Energy Profile and Surface Work Function of Vacuum Evaporated Molecular Films on Binary Semiconductor Surfaces

A.S. Komolov[1*], *E.F. Lazneva*[1], *S.A. Pshenichnyuk*[2], *V.S. Sobolev*[1], *O.V. Borshchev*[3], *S.A. Ponomarenko*[3]

[1]St. Petersburg State University
[2]Institute of Molecule and Crystal Physics, Subdivision of the Ufa Federal Research Centre of the RAS
[3]Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Sciences
*e-mail: a.komolov@spbu.ru

In this presentation some background information on electron spectroscopic studies of thin films of conjugated organic molecules on solid surfaces will be discussed. The focus will be made on monitoring of density of unoccupied states in conduction band and on monitoring of surface potential upon increasing the film thickness up to 10 - 20 nm. Changes of surface potential determine the height of the interfacial potential barrier. Binary semiconductor materials such as ZnO and CdS prepared by the atomic layer deposition (ALD) method are good candidates for substrate materials in potential device applications because of their uniform layer-by-layer structure. Thiophene/phenylene co-oligomers (TPCO), thienothiophene containing molecules and biphenyltetracarboxylic dianhydride molecules (Figure 1) were used for thermal deposition of thin and ultrathin layers of the molecular materials investigated. Investigations of the energy positioning of the maxima of unoccupied electronic states and of the process of the formation of the potential barrier between the film and the substrate were carried out by total current spectroscopy method (TCS).[1,2] Atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS) were used to determine the film surface roughness and atomic composition.

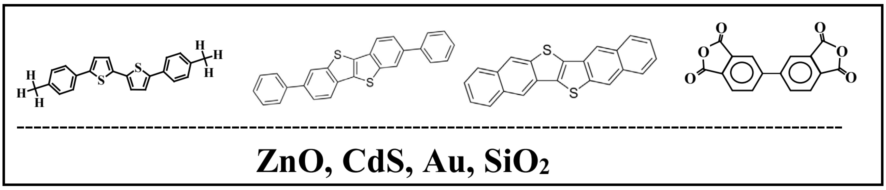


Figure 1. The schematics of the interfaces formed by organic films investigated on inorganic material surfaces.

The TCS investigation of TPCO on binary semiconductors was supported by RFBR grant 20-03-00026. The TCS investigation of the biphenyltetracarboxylic dianhydride films was supported by the Russian Science Foundation (project № 19-13-00021). TPCO and thienothiophene containing molecules were prepared under financial support of Ministry of Science and Higher Education of the Russian Federation (Contract 0071-2019-0006).The experiments were performed using the equipment of the Research park of St. Petersburg State University, centre for Physical methods of surface investigations.

---

[1] A.S. Komolov, E.F. Lazneva, S.N. Akhremtchik, N.S. Chepilko, A.A. Gavrikov. *J. Phys. Chem. C* 2013, **117**, 12633.

[2] A.S. Komolov, E.F. Lazneva, N.B. Gerasimova, Yu. A. Panina, V.S. Sobolev, A.V. Koroleva, S.A. Pshenichnyuk, N.L. Asfandiarov, A. Modelli, B. Handke, O.V. Borshchev, S.A. Ponomarenko. *J. Electron Spectr. Rel. Phenom.* 2019, **235**, 40.

O-19

Effect of Oligothiophene π-Bridge Length in D-π-A Star-Shaped Oligomers on Photophysics and Photovoltaic Performance in Organic Solar Cells

A.L. Mannanov[1,2*], *Yu.N. Luponosov*[1], *A.N. Solodukhin*[1], *P.S. Savchenko*[1], *B.A.L. Raul*[3], *N.M. Surin*[1], *M.S. Pshenichnikov*[3], *D.Yu. Paraschuk*[1,2], *S.A. Ponomarenko*[1]

[1]Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Sciences
[2]Faculty of Physics, Lomonosov Moscow State University
[3]Zernike Institute for Advanced Materials, University of Groningen
*e-mail: al.mannanov@physics.msu.ru

Donor-acceptor molecules having thiophene fragments as the π-bridge represent a promising class of materials for organic photovoltaics. However, the impact of the oligothiophene π-bridge length on physicochemical properties, photophysics, charge transport and photovoltaic performance of these materials has not been thoroughly addressed. Here we report on the comprehensive investigation of the series of star-shaped donor-acceptor oligomers (0T – 4T) having triphenylamine as a donor core linked through an oligothiophene π-bridge of variable length to the terminal hexyl-dicyanovinyl electron-withdrawing groups (Fig. 1). We found that variation of the π-bridge length from 0 to 4 thiophene units strongly impacts their properties such as the solubility, highest occupied molecular orbital energy, optical absorption and luminescence spectra, band gap, film morphology, phase behavior and molecular packing as well as the charge-carrier mobility[1]. As a result, the molecules showed different performance in single-component (SC OSCs) and bulk-heterojunction (BHJ OSCs) organic solar cells. The power conversion efficiency of the SC OSCs jumped from 0.06% for 1T to the remarkable 1.09% for 4T with π-bridge elongation, which is in a good agreement with their charge transport, generation and recombination properties, as supported by the ultrafast photoluminescence spectroscopy and Onsager model calculations. The SC OSCs showed relatively narrow responsivity spectra and operated also as spectrally-selective photodetectors. The photovoltaic performance in BHJ OSC with $PC_{71}BM$ as acceptor increased significantly with elongation of the π-bridge length from 0T to 2T; however, further elongation of the oligothiophene length did not promote performance in BHJ OSCs. The results obtained provide an insight on how to fine-tune and predict properties and photovoltaic performance of small molecules for organic solar cells.

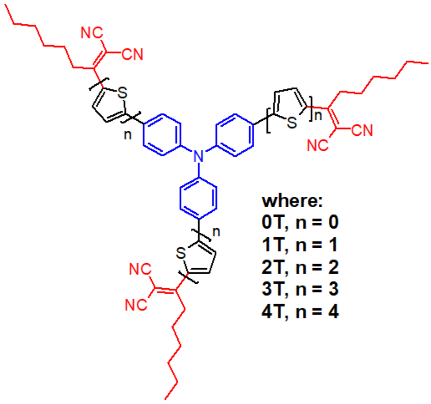


Fig. 1. Chemical structures of star-shaped D-π-A molecules 0T, 1T, 2T, 3T 4T

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

---

[1] Luponosov Yu.N. et al. *Materials Today Energy*. 2021. Under review.

Mesoscale Simulations of Photovoltaic Polymer Nanocomposites

P.V. Komarov[1,2], *D.V. Guseva*[1], *V.Yu. Rudyak*[3], *A.A. Gavrilov*[3], *V.A. Ivanov*[3], *S.-H. Tung*[4]
[1]A.N. Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia
[2]Tver State University, Tver, Russia
[3]M. V. Lomonosov Moscow State University, Moscow, Russia
[4] National Taiwan University, Taipei, Taiwan
*e-mail: pv_komarov@mail.ru

One of the potential alternatives to crystalline silicon solar cells is plastic solar cells (PSC) made of thin films based on polymer materials, which can be easily applied layer by layer onto flexible substrates of a large area using wet processing methods. Such devices give such promising advantages as ease of producing, possible recyclability, and relatively low cost. For the widespread of PSC in daily practice, it is necessary to achieve many properties, such as high power conversion efficiency, durability, and stability with prolonged exposure to temperature changes. When developing PSC, many polymeric materials need to be tested. The use of computer simulations can significantly facilitate the process verification of the properties of various polymers before their using in real devices.

This report discusses the problems of the design of computer models for investigations of the photoactive layer (PhL) of polymer solar cells. The PhL is a nanocomposite in which π-conjugated (semiconducting) polymers are used as matrices. Due to π-π stacking interactions, crystalline domains, which play an essential role in forming PhL properties, are formed in the structure of conjugated polymers. However, computer simulation methods have minimal possibilities for constructing models of polymeric materials, taking into account π-π interactions. This problem is especially acute for mesoscopic methods that allow the study of polymeric materials at relatively large lengths and time scales. We propose a method for taking into account π-π stacking interactions in mesoscale models and check it in the framework of the dissipative particle dynamics method. As a prototype of the polymer model, we use poly (3-hexylthiophene). We show that taking into account π-π stacking interaction leads to self-assembly of the polymer chains into large stacks with strong alignment. These stacks form lamellae, which is in good agreement with the known experimental data. The proposed methodology could be helpful in studies of conjugated polymer materials, especially in the design of PSC and other photovoltaic devices.

We also constructed the reverse-mapping procedure that makes it possible to create models of atomistic samples of PhL based on the final states of the mesoscopic models. This creates possibilities to construct the multiscale schemes for the simulation of the nanocomposites based on the conjugated polymers with various fillers to predict their thermophysical properties and thermal stability.

The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University with financial support from the Russian Foundation for Basic Research (Project No. 19-53-52004) and the Ministry of Science and Technology of Taiwan (Project MOST 108-2923-E-002-001-MY3).

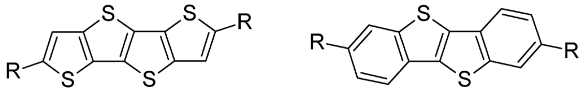
O-21

Synthesis and Properties of Thienoacenes for Organic Electronics

M.S. Skorotetcky[1]*, *O.V. Borshchev*[1], *A.Y. Sosorev*[2], *D.Y. Paraschuk*[2], *S.A. Ponomarenko*[1]

[1]Institute of Synthetic Polymer Materials RAS
[2]Moscow State University, Department of Chemistry
*e-mail: Skoroteckiy@ispm.ru

Organic electronics has been actively developed in recent years due to their advantages such as ease of processing, low manufacturing cost, and mechanical flexibility. Among a large variety of organic semiconductors, thienoacenes (Fig.1) have been widely investigated as promising organic semiconductors in high-performance OFETs. Fused-thiophene structure lead to unique properties, such as extensive conjugation, strong intermolecular S–S interactions, and rigid coplanar conjugated core, which contributes to attractive charge-transfer properties.[1]



TTA **BTBT**

Fig. 1. Structural formulas of tetrathienoacene (TTA) and benzothienobenzothiophene (BTBT) derivatives.

This work describes the synthesis, properties and application of new aliphatic and aromatic derivatives of TTA in various optoelectronic devices. The transformation of TTA in the Friedel-Crafts acylation reaction was studied for the first time.[2] The characteristics of organic field-effect transistors based on them, obtained by both solution and vacuum methods, have been investigated. The influence of dynamic disorder on charge transfer inside annelated organic semiconductors is also discussed.[3]

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

---

[1] Borshchev O.V, Skorotetcky M.S., Trukhanov V.A. et. al. *Dyes Pigm.* 2021, **185**, 108911

[2] Skorotetcky M.S., Borshchev O.V, Polinskaya M.S. et. al. *J. Mater. Chem. C* 2021, **submitted**

[3] Sosorev A.Y., Parashchuk O.D., Tukachev N.V. et. al. *Phys. Chem. Chem. Phys.* 2021 **accepted**

Ultrathin Hybrid Surface Coatings from Graphene Oxide and Polydiacetylenes for Fabricating Organic Photodiodes

E.A. Gusarova[1,2*], *A.I. Zvyagina*[2], *N.V. Kuzmina*[2], *A.E. Alexandrov*[2], *A.A. Averin*[2],
A.R. Tameev[2], *M.A. Kalinina*[2]

[1]Moscow State University, Faculty of Materials Science
[2]A.N. Frumkin Institute of Physical chemistry and Electrochemistry RAS
*e-mail: liisagus@mail.ru

Graphene-based materials are widely used in electronics and solar cells due to their large specific surface area, optical transparency, high mechanical strength, and excellent electrical conductivity. Such materials provide rational alternative to ITO electrodes in combination with electron transport and hole transport layers in polymer organic cells. Hybrid systems based on graphene oxide (GO), a cheap analog of graphene, and organic compounds are of particular interest in this respect. The main advantage of using hybrid systems over individual GO layers is the possibly of tuning the functions of the layer by using organic molecules with the appropriate characteristics.

In this work, we propose a simple one-step procedure for the preparation of ultrathin hybrid materials based on graphene oxide and 10,12-pentacosadiynoic acid (PDA). Strong interactions between these components leads to a synergy of properties of the components in the resulting material. To obtain ultrathin PDA/GO coatings, a silicon or quartz substrate was dipped into the GO hydrosol. A thin layer of PDA in a volatile solvent was deposited onto the surface of the hydrosol to allow formation of the PDA/GO adsorption layer. The layer was deposited onto the solid supports by vertical transferring across the interface. The as-formed PDA/GO composites were irradiated by UV light at 254 nm to polymerize the PDA monomers. To increase the electrical properties of the resulting layer, the solid-supported coatings were then heated by microwave irradiation for reduction of GO. The presence of both components in the films was confirmed by the appearance of characteristic bands of PDA and reduced GO (rGO) in the absorption spectra. The uniformity of the PDA distribution over the rGO surface was confirmed by SEM as well as by the surface mapping using Raman spectroscopy. The thickness of such coatings about 10 nm was determined by AFM. AFM images show that PDA polymer overlaps the gaps between the rGO sheets, thereby "healing" the defects in the rGO monolayer. The measurements of electric characteristics of PDA/rGO hybrids showed an increase in conductivity by more than 6 times (down to 46 $S\bullet cm^{-1}$) compared to that of the rGO monolayers. This increase is a consequence of a decrease in the number of defects in the system reducing the contact resistance. The integration of these hybrid layers into the ITO/ GO+PDA/ C_{60} / BCP/ Al solar cell bottom-up architecture led to the photovoltaic effect. The ultrathin PDA/GO layer in the cell performs several functions - a photosensitizer, a hole transport layer, and a diode. It is important to note that the photovoltaic effect was observed even with a relatively low absorption of photons in an ultrathin PDA layer (8 nm): the short-circuit current and open-circuit voltage in this system are 0.3 μA and 0.2 V, respectively. The results suggest that hybrid ultrathin systems based on GO and organic conducting layers can be potentially promising alternative for the ITO electrodes in nanoelectronics and photovoltaic devices.

This work was supported by the Russian Science Foundation (project № 20-13-00279).

O-23

Hot Carrier Cooling Dynamics in Lead Halide Perovskite Nanocrystals Revealed by Ultrafast Multi-Pulse Spectroscopy

B. Carwithen[1], T. Hopper[1], F. Krieg[2], M. Bodnarchuk[2], M. Kovalenko[2], A. Bakulin[1**]*

[1]Department of Chemistry, Imperial College London
[2]Department of Chemistry and Applied Biosciences, ETH Zurich
*e-mail: b.carwithen19@imperial.ac.uk
**e-mail: a.bakulin@imperial.ac.uk

The relaxation of hot (above-gap) carriers in semiconductors is responsible for major efficiency losses in present-day solar cells, and involves a complex interplay between carrier-carrier and carrier-phonon coupling. Unravelling the mechanisms of cooling is therefore an essential step for both understanding and developing emerging photovoltaic materials. Perovskite nanomaterials are an exciting class of compounds because they offer facile and broad optoelectronic tunability by size, dimensionality and composition. Here, we aim to elucidate the effects of these properties on carrier cooling by employing ultrafast pump-push-probe spectroscopy. This narrow-band three-pulse technique allows cooling to be isolated from a melee of other excited state processes, while also allowing independent control over the hot and cold (band-edge) carrier subpopulations. These experiments show that while carrier cooling is generally indifferent to nanocrystal size in moderately confined systems,[1] intriguing results are obtained upon altering the shape of the nanocrystal, and are also influenced greatly by material composition.[2]

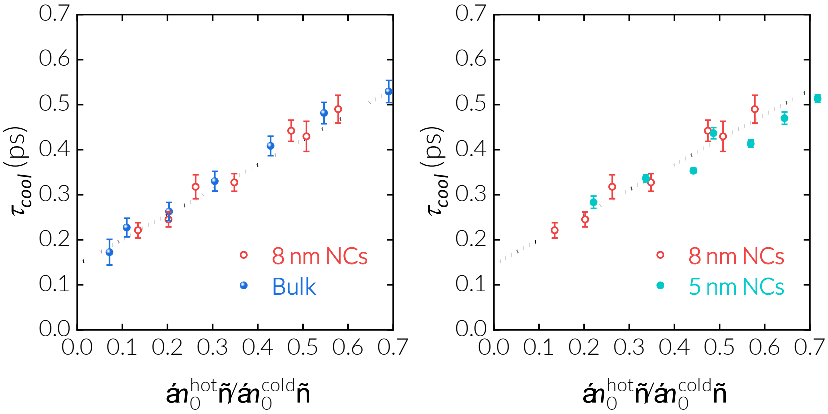


Figure 1: Hot carrier density-dependent cooling times for bulk, and nanocrystalline $CsPbBr_3$

This work was supported by ERC (639750) and EPSRC.

---

[1] T. R. Hopper, A. Gorodetsky, A. Jeong, F. Krieg, M. I. Bodnarchuk, M. Maimaris, M. Chaplain, T. J. Macdonald, X. Huang, R. Lovrincic, M. V. Kovalenko and A. A. Bakulin, *Nano Lett.*, 2020, **20**, 2271–2278.

[2] T. R. Hopper, A. Gorodetsky, J. M. Frost, C. Müller, R. Lovrincic and A. A. Bakulin, *ACS Energy Lett.*, 2018, **3**, 2199–2205

Poster presentations

P-1

The Compact Hardware Platform for Multiple Electrochemical and Metal-Oxide Sensors Evaluation

A.A. Abramov[1*], *D.S. Anisimov*[1], *A.A. Trul*[1], *E.V. Agina*[1], *S.A. Ponomarenko*[1]

[1]Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Sciences
*e-mail: abramov@ispm.ru

Systems with multiple gas sensors attract interest in such fields as air quality control, exhaled breath analysis, food and drinks quality estimation, electronic nose systems, etc. Several types of gas sensors might be used in such kinds of devices.[1] Electrochemical and metal-oxide sensors (MOS) are a common solution today in portable gas sensing applications due to their low power consumption, small size, and data acquisition simplicity.[2] A system including as well highly sensitive OFET-based sensors could combine a broad spectrum of detectable gases, high selectivity to target gases and ultra-low detection limits.

The aim of this work was the development of a modular hardware platform, which would allow to simultaneously acquire signals from a set of different electrochemical, metal-oxide, and other resistive-type sensors and being applicable in a gas chamber and atmosphere. Electrochemical cells designed for various gases require different measurement conditions, such as bias voltage and load resistance, which can be varied for optimal performance. For this purpose, tunable analog-frond-end (AFE) integrated circuits (IC) are suitable. Integrated circuits of this kind incorporate a potentiostatic circuit and a set of switches and multiplexers, which allow discretely changing the parameters of the circuit. Since the MOS and organic resistive sensors respond to gases with a change of resistivity, the AFE circuit can be reconfigured to the two-electrode mode. Known bias voltage allows calculating the sensor's resistance from the measured current. The bias voltage variation is important since was shown to play role in the sensor's performance.[3]

This approach allows decreasing complexity and the size of the printed circuit board (PCB), saves cost and time by excluding analog debugging, increases the immunity of the circuit to interferences and contaminants by reducing trace length and the number of soldered joints. Configurability of the analog circuit enables adapting circuit to different cells from software and producing boards with an identical set of electronic components suitable for different tasks.

The device developed consists of six analog front-end IC's, a six-channel sigma-delta analog-to-digital converter, microcontroller unit, linear voltage regulators, and voltage references. Custom-designed two-layer PCB allows installing sockets to fit in electrochemical cells by SPEC Sensors or by SGX Sensortech. Metal-oxide and other sensors in TO or SMD package can be plugged in with the use of custom converting PCB. The board also allows the connection of four sensors with I2C interface. All electronic components are placed on one side of the board opposite to sensors to allow flange-like mounting to the wall of some enclosure or gas chamber. Data acquisition is performed via USB interface or attachable Bluetooth or WiFi module. The total power consumption of the circuit does not exceed 250 mW with six electrochemical cells and can raise to two watts with six MOS-sensors installed.

The device developed is a versatile platform for building an electronic nose based on an array of sensors of different types and target gases.

This work was supported by Ministry of Science and Higher Education of the Russian Federation (Contract 0071-2021-0003).

---

[1] D. Karakaya et al, *International Journal of Automation and Computing*, 2020, **17**(2), 179.

[2] Wojciech Wojnowski el al, *Sensors* 2017, **17**(12), 2715

[3] Sardar M. Ayub Durrani, *Sensors* 2006, 6(9), 1153-1160.

P-2

Novel Thiophene-Containing Donor Small Molecules with Various Topology: Synthesis, Properties and Application in Organic Solar Cells

D.O. Balakirev[1*], *N.K. Kalinichenko*[1], *P.K. Sukhorukova*[1], *Yu.N. Luponosov*[1],
E.A. Svidchenko[1], *S.M. Peregudova*[2], *A. L. Mannanov*[1,3], *P.S. Savchenko*[1],
D.Yu. Paraschuk[1,3],*S.A. Ponomarenko*[1]

[1]Enikolopov Institute of Synthetic Polymeric Materials, Russian Academy of Sciences
[2]Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences
[3]Lomonosov Moscow State University, Faculty of Physics & International Laser Center
*e-mail: balakirev@ispm.ru

Organic photovoltaics is a dynamically developing field. The search and development of new functional materials for organic solar cells (OSC) remains an urgent task.

Here we report on an efficient synthesis and comprehensive investigation of properties of novel thiophene-containing donor-π-acceptor small molecules with linear and star-shaped topology. These molecules, which containing different electron-withdrawing groups (either alkyl-dicyanovinyl or alkyl-cyanoacetate ones), conjugated through oligothiophene π-spacer with different electron-donating cores based on either benzotriindole, benzodithiophene or thiophene were synthesized in high yields. Their thermal, optical, and electrochemical properties, as well as the phase behavior were studied and compared. The analysis of the results obtained made it possible to establish a number of significant structurally inherent regularities and their influence on the efficiency of photovoltaic devices in which the obtained small molecules were used as p-type organic semiconductor materials.[1,2,3]

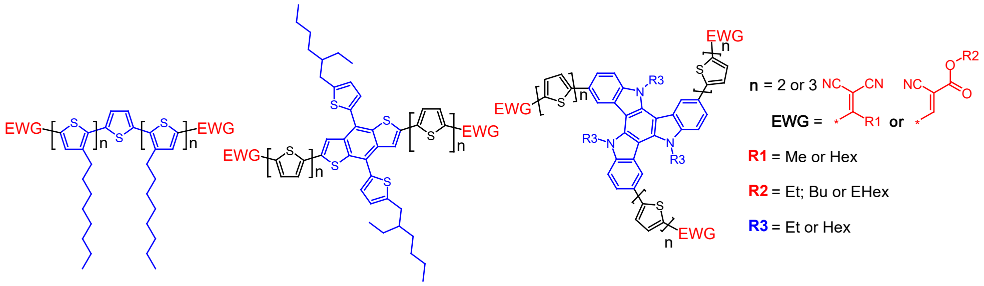


Figure 1. General chemical structures of thiophene-containing donor small molecules

The work was performed with the financial support by a grant from the Russian Science Foundation (project №19-73-10198).

---

[1] Guo J., Balakirev D.O., Gu C., Peregudova S.M., Ponomarenko S.A., Liu Z., Luponosov Yu.N., Min J., Lei A. *Dyes and Pigments*, 2020, **175**, 108078.

[2] Balakirev D.O., Luponosov Yu.N., Mannanov A.L., Savchenko P.S., Minenkov Y., Paraschuk D.Yu., Ponomarenko S.A. *Dyes and Pigments*, 2020, **181**, 108523.

[3] Kalinichenko N.K., Balakirev D.O., Savchenko P.S., Mannanov A.L., Peregudova S.M., Paraschuk D.Yu., Ponomarenko S.A., Luponosov Yu.N. *Dyes and Pigments*, 2021, **194**, 109592.

New Organic Luminophores for Optoelectronics

O.V. Borshchev[1*], *M.S. Skorotetcky*[1], *N.M. Surin*[1], *S.A. Ponomarenko*[1,2]

[1] Enikolopov Institute of Synthetic Polymeric Materials RAS
[2]Moscow State University, Department of Chemistry
*e-mail: borshchev@ispm.ru

During the last years, the number of light-harvesting luminescent dendritic molecules has increased rapidly. One of the most interesting features of these molecules is a possibility of incorporation of different chromophores within one molecule that can lead to an intramolecular directional energy transfer from their peripheries to the center. Recently we have developed a new class of highly efficient luminescent materials with unique properties - nanostructured organosilicon luminophores (NOLs).[1,2,3] These are branched molecules, where two types of organic chromophores are connected to each other via silicon atoms, which brake the conjugation between them and fix them specifically in the space.[4,5,6] NOLs possess several advantages: absorption in a wide optical spectral region; 5–10 times higher absorption cross-sections than those of the best low molar weight organic luminophores; very high photoluminescence quantum yield; luminescence spectra in the defined wavelength region; short luminescence lifetime. Photoluminescence study of the NOLs has shown an intramolecular energy transfer with the efficiency up to 99% and luminescence quantum yield up to 95% in various spectral regions. Optical and thermal properties of the NOLs were compared with the properties of the model linear oligomers.[7] It should be noted that combination of different chromophores in NOLs allows tuning their emission wavelengths in a wide spectral region, which open possibilities for their wide application as spectral shifters – convertors of the emission with the energy of high frequency photons (140–400 nm) into emission in the visible spectral range (400–700 nm).[8]

We applied NOLs as organic luminophores for manufacturing scintillation and wavelength shifting polymer fibers.[9] A blue and a green emitting prototype fibre were produced and characterised in terms of attenuation length, ionisation light yield, decay time and tolerance to x-ray irradiation. Both the blue and the green prototype fibres show a very short decay time constant and mark to our knowledge new records. The GPF-19-1 prototype fibre is about a factor 6 faster than the SCSF-3HF fibre produced by Kuraray and about two times faster than the green BCF-20 fibre produced by Saint-Gobain Crystals.

The new NOLs used in various devices of organic photonics and electronics, such as spectral shifting fibers,[9] organic light-emitting diodes (OLEDs),[10] CIGS photovoltaic devices.[11] NOLs are commercialized by a startup Limited Liability Company "Luminescent Innovative Technologies" (LumInnoTech LLC, www.luminnotech.com).

This work was supported by RFBR (№18-29-17006MK).

---

[1] S.A. Ponomarenko, N.M. Surin, O.V. Borshchev, at. al. *Scientific Reports* 2014, **4**, 6549.
[2] T.Yu. Starikova, N.M. Surin, O.V. Borshchev, at. al., *J. Mater. Chem. C,* 2016, **4**, 4699.
[3] S.A. Ponomarenko, N.M. Surin, O.V. Borshchev, at. al., *Proc. SPIE*, 9545, 2015, 954509-1.
[4] O.V. Borshchev, S.A. Ponomarenko, at. al., *Organometallics*, 2007, **26**, 5165.
[5] Yu.N. Luponosov, S.A. Ponomarenko et al., *Chem. Mater.* 2009, **21**, 447.
[6] O.V. Borshchev, Y.N. Luponosov, et al., *Russ. Chem. Bull.*, 2010, **4**, 781.
[7] M.S. Skorotetcky, E.D. Krivtsova, at. al., *Dyes and Pigments* 2018, **155**, 284–291.
[8] D.Y. Akimov, O.V. Borshchev, S.A. Ponomarenko, at. al., *NIM A*, 2012, **695**, 403-406.
[9] O. Borshchev, A.B.R. Cavalcante, L. Gavardi, O. Shinjie at. al., *JINST* 2017. **12**. P05013
[10] Y.N. Luponosov, N.M. Surin, at. al., *Org. Photonics Photovolt.*, 2015, **3**, 148-155
[11] T. Uekert, A. Solodovnyk, at. al., *Sol. Energy Mat. Sol. Cells*, 2016, **155**, 1-8.

Tuning the Optoelectronic Properties of Sulfurated Carbazole Derivatives: the Case of the Bisbenzothienocarbazole Core

R. Bujaldón[1,2], *J. Puigdollers*[3], *D. Velasco*[1,2*]

[1]Departament de Química Inorgànica i Orgànica, Universitat de Barcelona
[2]Institut de Nanociència i Nanotecnologia (IN^{2}UB)
[3]Departament d'Enginyeria Electrònica, Universitat Politècnica de Catalunya
*e-mail: d.velasco@ub.edu

Considering the potential of the 14*H*-bis[1]benzothieno[3,2-*b*:2',3'-*h*]carbazole core as a hole-transporting semiconductor, in this study we synthesized a set of two derivatives possessing a different alkylation patterning. The followed synthetic route[1] involved various sulfurated molecules based on the carbazole scaffold. Unexpectedly, the chromophores containing a sulfoxide group enhanced their blue fluorescence with respect to the nearly non-emitting sulfur counterparts. Regarding this, we could characterize the relationship between their chemical structure and their emission as an approach for future applications. Considering the performance in Organic Thin-Film Transistors (OTFTs), both bisbenzothienocarbazole derivatives displayed p-type characteristics, with charge mobility values up to 1.1×10^{-3} cm^2 V^{-1} s^{-1}. As reported for another carbazole-based constructions[2], the role of the alkylation patterning was a key factor to modulate both the intermolecular interactions and, consequently, the performance of the final devices.

This work was supported by the Ministerio de Economía y Competitividad (project № FUNMAT-PGC2018-095477-B-I00).

---

[1] Gao P., Feng X., Yang X., Enkelmann V., Baumgarten M., Müllen K. *J. Org. Chem.* 2008, **73**, 9207-9213.

[2] Reig M., Bagdziunas G., Ramanavicius A., Puigdollers J., Velasco D. *Phys. Chem. Chem. Phys.* 2018, **20**, 17889-17898.

P-5

Modelling of Charge Transport in Polymers with Imbedded High-Ordered Nanoscale Regions

Ya.V. Burdakov[1*], *V.R. Nikitenko*[1]

[1]National Research Nuclear University "MEPhI" (Moscow Engineering Physics Institute)
*e-mail: burdakov_y@mail.ru

Charge transport, which characterized by mobility in general, is one of the key physical processes behind the operation of electronic devices. The active semiconductor layer in such devices is typically a thin (about 100 nm) film. In a disordered polymer, macromolecules can be oriented in a rather chaotic manner (amorphous phase), but they can be oriented more or less in parallel to each other, forming the aggregated nano-scale regions with reduced disorder, see Figure 1, which will be referred below as the crystallites. The aim of this work is the theoretical analysis of charge mobility in thin 2-phase organic layers by means of Monte-Carlo simulations and analytic modelling. Energy distribution of states in both phases is Gaussian, the variance is σ_1 and $\sigma_2 = \sigma_1/3$, respectively, the mean energy of states of a crystallite phase is shifted down relative to the same of amorphous phase by the energy E_t. Hopping occurs faster inside crystallites due to reduced disorder and weaker localization.

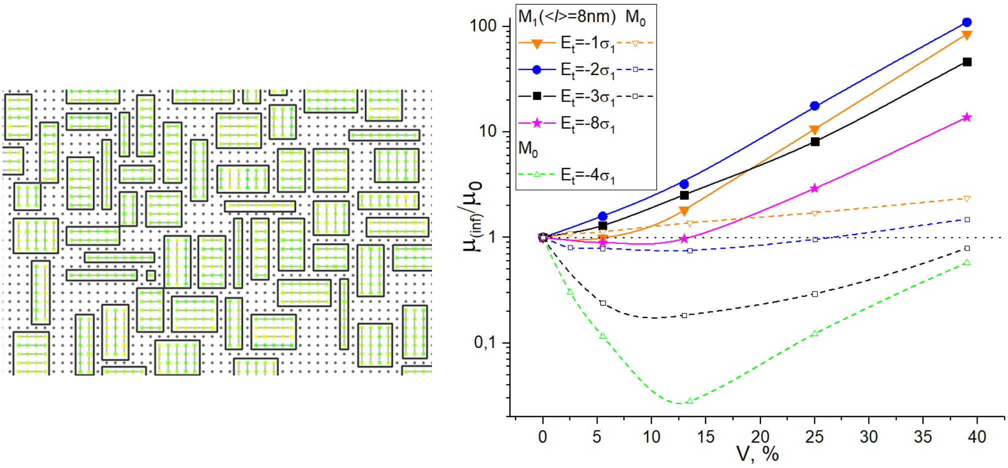


Figure. 1 Left: Illustration of a two-phase structure, where the dots indicate the amorphous phase and the rectangles indicate the crystallites. Right: the mobility depending on the fraction of a sites of the second phase, *V*. <*l*> is a mean size of crystallites. M_1 indicates the structure of a left figure and M_0 describes a structure where the energy distribution is the same but the sites of the second phase randomly distributed over the entire volume of the material (2-Gaussian amorphous material).

Calculations performed for a room temperature, $\sigma_2 = 2.13kT$. Modeling showed a strong effect of the morphology (M_1 or M_0) on the mobility, see the right part of the figure. The conditions for maximum mobility have been determined. An analytic model based on the multiple-trapping approach[1] can describe these peculiarities of the mobility qualitatively.

This work was supported by the VW Foundation within the project "Understanding the dependence of charge transport on morphology in organic semiconductor films".

---

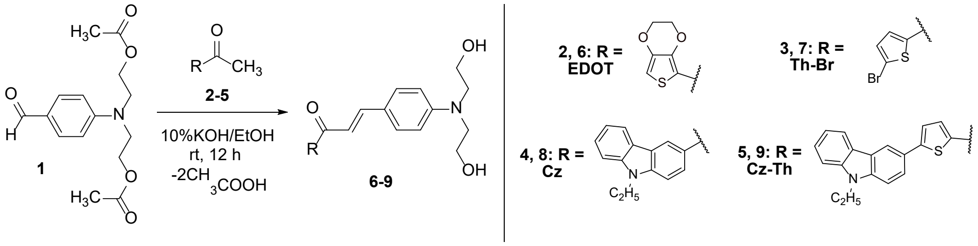
[1] R. Saxena, V. R. Nikitenko, I. I. Fishchuk, Ya. V. Burdakov, Yu. V. Metel, J. Genoe, H. Bässler, A. Köhler, and A. Kadashchuk. *Phys. Rev.B* 2021 **103**, 165202.

P-6

Novel Chalcones Containing 4-*Bis*(2-Hydroxyethyl)Aminophenyl Moiety: Synthesis and Optical Properties

A.N. Chukhlantseva[1,2*], *A.N. Vasyanin*[2], *M.V. Dmitriev*[2], *E.V. Shklyaeva*[2], *G.G. Abashev*[2]
[1]Department of Technical Chemistry of the Ural Branch of the RAS
[2]Perm State National Research University
*e-mail: ignashevich.anna@mail.ru

Chalcones containing simultaneously ED and EW groups present a class of chromophores, exhibit photophysical and photochemical properties which make them attractive as materials for optoelectronic devices[1] and materials for nonlinear optics (NLO).[2] At the same time these compounds are easy to prepare. *N,N*-Disubstituted anilines are often used as donor fragments in such structures; it is known that chromophores containing terminal *N,N*-di(ω-hydroxyalkyl)aniline moieties demonstrate the pronounced fluorescent properties and, at the same time, hydroxy groups can be replaced by alkoxy groups or halogen atoms.[3] Claisen-Schmidt condensation of aldehyde **1**[**4**] with methyl ketones **2-5** has given rise to the chalcones **6-9** containing terminal hydroxy groups (Scheme 1).



Scheme 1. Synthesis of chalcones, including 4-*bis*(2-hydroxyethyl)aminophenyl fragments

The resulting chalcones **6-9** have the bright fluorescence both in solutions and in a solid state. UV absorption and emission spectra of the obtained chalcones have been investigated. The highest value of ahe Stokes shift and fluorescence quantum yield belong to chalcone **7** (97 nm, 44.3%) in $CHCl_3$ as a solvent. The maximum value of the extinction coefficient is inherent to chalcone **8** (31110), and the narrowest bandgap (2.32 eV) - to chalcone **9**. The change of a solvent is usually accompanied by the changes in polarity, dielectric constant, or in polarizability; this consequently affects the main and the excited state in different ways[5], that's why the UV absorption and fluorescence spectra of all synthesized compounds were estimated in the solvents of different polarity. All chacones are characterized by positive solvatochromism, exhibited by their UV absorption and fluorescence spectra.

The reported study was funded by RFBR and Perm Territory according to the research project № 19-43-590014

---

[1] Ali M. K. M., Elzupir A., et al. *Optik*. 2017, **145**, 529–533.

[2] Abegão L. M. G., Fonseca R. D., et al. *Chem. Phys. Lett.* 2016, **648**, 91–96.

[3] Bourson J., Valeur B. *J. Phys. Chem.* 1989, **93**(9), 3871–3876.

[4] Yuquan S., Yuxia Z., et al. J. *Chem. Soc. Perkin Trans. I.* 1999, **24**, 3691–3695.

[5] Gülseven Sıdır Y.,Sıdır İ. *Spectrochim. Acta A Mol. Biomol. Spectrosc.* 2013, **102**, 286–296.

Synthesis of New Conjugated Polymers Based on Triphenylamine, Containing Electron-Withdrawing Groups

I.A. Chuyko[1*], *A.N. Solodukhin*[1], *S.M. Peregudova*[2], *Yu.N. Luponosov*[1], *S.A. Ponomarenko*[1,3]
[1]Institute of Synthetic Polymeric Materials of RAS, Moscow, Russia
[2]Institute of Organoelement Compounds of RAS, Moscow, Russia
[3]Chemistry Department, Lomonosov Moscow State University, Moscow, Russia
*e-mail: chuyko@ispm.ru

Polymers based on triphenylamine (TPA) are of great interest to researchers. Such materials demonstrate a combination of high thermal and electrochemical stability with good hole-transport properties. The introduction of a TPA block into macromolecules helps to suppress intermolecular aggregation and reduce the tendency to crystallization. As a result, such materials have good solubility and, as a rule, are amorphous and have high glass transition temperatures. The attachment of various electron-withdrawing groups to such polymers allows fine tuning of the electrochemical and optical properties of the resulting materials. Such advantages of triphenylamine-containing polymers make it possible to use them as an active layer in various devices of organic electronics and photonics[1, 2].

In this work, we report on the design, synthesis and complex study of new D-A conjugated polymer based on triphenylamine with electron-withdrawing hexyldicyanovinyl groups (Figure 1). The purity and chemical structure of the precursors and the final polymer were studied by gel permeation chromatography and ^{1}H NMR spectroscopy. The electrochemical, thermal, and optical properties of the obtained polymer were studied using cyclic voltammetry, differential scanning calorimetry, thermogravimetric analysis, and ultraviolet spectroscopy. Comparison of the properties of the obtained polymers with different molecular weights with each other and with the closest low-molecular-weight analog will reveal the influence of the type of molecular organization on the properties of such compounds.

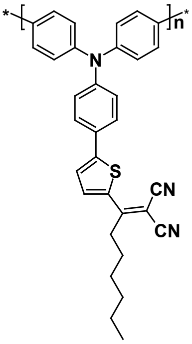


Figure 1. Structural formula of a conjugated polymer based on triphenylamine.

This work was supported by RFBR (project № 20-73-00266).

---

[1] Iwan A., Sek D. *Progress in Polymer Science*. 2011, **36**, 1277-1325.

[2] Rybakiewicz, R., Zagorska, M., Pron, A. *Chemical Papers*. 2016, **71**(2), 243-268.

Synthesis and Properties of Novel Liquid Luminescent Chromophores Based on Organic π-Conjugated Oligomers

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

[1]Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Science
*e-mail: dyadischev_iv@ispm.ru

Liquid organic luminophores are a relatively new and class of materials, which have high processability owing to their fluidic nature and efficient fluorescence in pristine state.[1] However, the structure-property relationships of such compounds remain poorly understood. In addition, they exhibit luminescence in a limited short-wavelength region of the spectrum. The introduction of electron-withdrawing units and solubilizing groups of various nature into these molecules allows fine tuning of the properties of the obtained materials. The absence of aggregation and the need to use solvents increases the manufacturability and environmental friendliness of the processes of manufacturing devices based on such functional materials and opens up new areas of their application.

In the course of this work, new oligomers based on 2,2'-biphenyl-4,4'-diylthiophene with linear and branched alkyl, trialkylsilyl with different lengths and branching of alkyls and alkyloligodimethylsiloxane solubilizing groups were synthesized to study the influence of the type, length and branching degree of solubilizing groups on thermal stability, aggregate state, phase behaviour, rheology and optical properties.[2] When the most effective solubilizing group for liquefaction was identifying, the series of novel liquid benzothiadiazole-based luminophores containing phenylene or thiophene units with terminal trihexylsilyl groups on each side of the central core were synthesized. The high purity and specified structure of all the compounds obtained was proved by a complex of modern research methods. The influence of the nature, length and branching of the solubilizing groups and type of π-conjugated core on the optical properties, rheology, phase behavior and thermal stability of luminophores has been studied. Based on this study, the most suitable group was selected to reduce aggregation in a condensed state, using which new liquid luminophores of oligomeric structure were obtained, emitting light in various ranges of the visible spectrum.

This work was supported by the Russian Foundation for Basic Research (grant № 18-33-20224). NMR and UV–vis spectra were recorded using the equipment of Collaborative Access Center 'Center for Polymer Research' of Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Sciences with the financial support from the Ministry of Science and Higher Education of the Russian Federation (Contract 0071-2021-0005).

---

[1] Fengniu Lu and Takashi Nakanishi., *Adv. Optical Mater.* 2019, **1900176.**

[2] Yuriy N. Luponosov, Dmitry O. Balakirev, Ivan V. Dyadishchev, Alexander N. Solodukhin, Marina A. Obrezkova, Evgeniya A. Svidchenko, Nikolay M. Surin, Sergei A. Ponomarenko., *J. Mater. Chem. C*, 2020, **8**, 17074-17082

P-9

Effect of Molecular Doping on Charge Transport and Electroluminescence of 2D Organic Semiconductors

R.S. Fedorenko[1,2*], *A.V. Kuevda*[1,2], *O.V.Borshchev*[2], *S.A. Ponomarenko*[2], *D.Yu. Paraschuk*[1,2]

[1]Faculty of Physics, Lomonosov Moscow State University
[2]Institute of Synthetic Polymer Materials RAS
[*]e-mail: roman96233@yandex.ru

Recent progress in organic field-effect transistors (OFET) based on 2D single crystals[1] stimulates the interest to 2D organic light-emitting transistors (OLET). BTBT-based small molecules show high charge-carrier mobilities in OFET,[2] but they are weakly luminescent. Addition of an appropriate molecular dopant acting as a luminophore could be a way to improve the luminescent properties and keep efficient charge transport in an OLET material.

In this work, we use BTBT-based molecules (2,7-bis(4-decylphenyl)[1]benzothieno[3,2-b][1]benzothiophene) (Dec-P)$_2$-BTBT. 2D (Dec-P)$_2$-BTBT films with lateral dimensions in the range of 300–600 μm were grown on silicon substrates. Upon the addition of 1% dopant with the tetrathienoacene (TTA) core, 4-hexyl-phenyl (Hex-P)$_2$-TTA), the lateral dimensions of the films increased to 2–3 mm (Figure 1 a). Figure 1b shows an image of a typical OFET fabricated on a silicon substrate and its transfer characteristic is shown in Figure 1c. The hole mobility in monolayer OFETs based on pristine and doped (Dec-P)$_2$-BTBT in the linear regime was in the range 0.6–0.8 and 0.1–0.2 cm^2/Vs, respectively. Using pure and doped (Dec-P)$_2$-BTBT 2D films as active layers, we fabricated OLET with gold electrodes. For doped devices, we recorded light emission, which was not observed with pure (Dec-P)$_2$-BTBT. As a result, we have found that the addition of dopant improves the growth of 2D films and electroluminescent properties but moderately reduces the charge-carrier mobility.

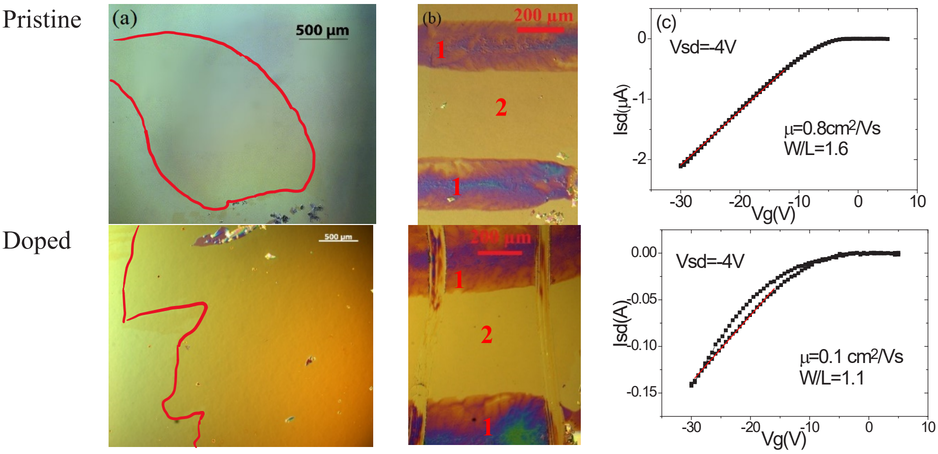


Figure 1. Optical image of (Dec-P)$_2$-BTBT monolayer (underlined by red line) (a); OFET optical image showing source and drain contacts (1), which were plotted with PEDOT:PSS; (Dec-P)$_2$-BTBT film (2); OFET transfer characteristics in the linear regime (c).

This work is supported by Russian Science Foundation (project 18-12-00499) and Theoretical Physics and Mathematics Advancement Foundation «BASIS».

---

[1] Bruevich V., et al., *ACS Appl. Mater. Interfaces* 2019, **11**, 6315–6324.

[2] Minemawari H., et al., *Nature* 2011, **475**, 364–367.

P-10

Impact of the Chemical Purity on the Semiconductor Properties of 2D Single Crystals

K.N. Kuklin[1*], *R.S. Fedorenko*[1,2], *A.V. Kuevda*[1,2], *O.V.Borshchev*[2], *S.A. Ponomarenko*[2],
A.Yu. Sosorev, D.Yu. Parashchuk[1,2]

[1]Faculty of Physics, Lomonosov Moscow State University
[2]Institute of Synthetic Polymer Materials RAS
[*]e-mail: kostyakuklin122@gmail.com

2D organic semiconductor single crystals are promising materials for organic field-effect devices.[1] In this contribution, we study the impact of chemical impurities on charge transport in 2D organic semiconductor single crystals. In 3D materials, it is known that they can act as traps, cause structural distortions in the crystal lattice, and affect the optical properties. We focus here on impurities that are detected by photoluminescence (PL) spectroscopy and reveal themselves as an intra bandgap PL band. We assume that the impurity is a self-dopant — a longer conjugated molecule appeared as a by-product of chemical synthesis.[2] We used oligothiophenphenylene 1,4-bis (5'-hexyl-2,2'-bithiophene-5-yl) benzene (DH-TTPTT) with a self-doping level of 0.01% and 0.2% evaluated from PL measurements in solutions. The solution was applied by spin coating at a concentration of 0.1–0.6 g/l. The top electrodes of the organic field-effect transistors (OFETs) were plotted by using PEDOT:PSS. The measured OFET data show that the hole mobility values for the self-doping levels coincided within the measurement accuracy limits (Fig. 1a); however, the threshold voltages slightly differ (Fig. 1a).

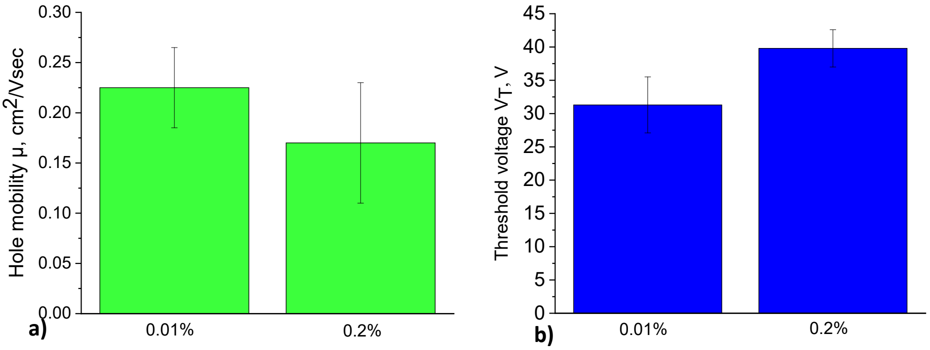


Fig 1. OFET data for different self-doping level: maximum hole mobilities (a) and the average threshold voltages (b).

The PL data in the 2D crystals showed that the self-dopant is incorporated in the crystals. Therefore, the presence of the self-doping at the level 0.2% and below does not affect the charge carrier mobility in 2D OFETs, but weakly impact the threshold voltage. Therefore, we conclude that the self-dopant species seemingly act as deep traps for charge carriers. From DFT calculations of various possible self-dopants and experimental PL spectra of the self-doped samples we suggest that the most plausible self-dopant is the starting molecule with oxidized thiophenes (sulfones).

This work is supported by Russian Science Foundation (project 18-12-00499).

---

[1] Bruevich V.V. et al. *ACS Appl. Mater. Interfaces*, 2019, **11**(6), 7
[2] Parashchuk O.D. et al. *Adv. Funct. Mater,* 2018, **28**(21), 46

Synthesis of Novel Donor-Acceptor Triazatruxene-Based Isomers End-Capped with Alkyldicyanovinyl or Cyanoacetate Groups

N.K. Kalinichenko[1*], *P.K. Sukhorukova*[2], *D.O. Balakirev*[1], *Yu. N. Luponosov*[1], *S.A. Ponomarenko*[1]

[1] Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Sciences,
[2] Department of Chemistry, M. V. Lomonosov Moscow State University
*e-mail: kalinichenko@ispm.ru

Triazatruxenes are widely used type of compounds for organic and hybrid electronics because of their good optical properties, high solubility due to the three nitrogen-carried alkyl sidechains and relatively simple and low-cost synthesis.[1,2,3,4] A star-shaped architecture with conjugated arms provides well-defined molecular structures with the excellent film-forming properties, intramolecular charge transfer and self-assembly.[5]

The alternating donor-acceptor approach allows to fine-tune physical and chemical characteristics of the organic conjugated polymers and small molecules by varying the electron-rich and electron-deficient units, the length of the π-conjugated spacer between them, and by introducing additional solubilizing alkyl groups.[6]

Here a series of triazatruxene-based isomers with terminal electron withdrawing groups on each side of the central core were synthesized. All precursors and the target compounds were characterized by ^{1}H and ^{13}C NMR spectroscopy and size exclusion chromatography in an individual state. Optical, thermal and electrochemical properties of molecules were studied and compared. The obtained triazatruxenes are promising candidates for organic and hybrid photovoltaics.

This work was supported by the Russian Science Foundation (grant №19-73-10198). NMR analysis was performed in Collaborative Research Center "Center for Polymer Research" of ISPM RAS supported by Ministry of Science and Higher Education of Russian Federation (topic No. 0071-2021-0005).

---

[1] T. Bura, N. Leclerc, R. Bechara, et al., *Adv. Energy Mater.*, **2013**, 3, 1118.

[2] I. Bulut, P. Leveque, B. Heinrich, et al., *J. Mater. Chem. A*, **2015**, 3, 6620.

[3] D.O. Balakirev, Yu.N. Luponosov, A.L. Mannanov, et al., *Dyes Pigm.*, 2020, 108523.

[4] A.N. Solodukhin, Yu.N. Luponosov, et al., *Energies*, **2021**, 14(12), 3596.

[5] X.-C. Li, C.-Y. Wang, W.-Y. Lai, et al., *J. Mater. Chem. C*, **2016**, 4, 10574.

[6] D.R. Kil, C. Lu, J. Ji, Kim, et al., *Nanomaterials*, **2020**, 10, 936.

P-12

A New Approach for Obtaining of Functional Dimethylsiloxane Matrices for Dielectric Elastomer Actuators

A.G. Khmelnitskaya [1], A.A. Kalinina [1], E.V. Agina [1], S.A. Ponomarenko [1], A.M. Muzafarov [1,2]

[1]Institute of Synthetic Polymer Materials RAS
[2]A.N.Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences
*e-mail: akazaeva95@gmail.com

The design of materials for dielectric elastomer actuators is an urgent problem over recent years. Such materials must have a set of properties: high dielectric constant, low conductivity, low dielectric loss factor, low Young's modulus.[1] Silicones have firmly taken the place of the most used materials for designing actuators based on them.[2] Nevertheless, they have a low dielectric constant (ε '= 2.3) and, as a consequence, high voltages, which limits their use. The solution to this problem is the chemical modification of the polysiloxane matrix with polar groups.[3,4] The development of modern methods of chemistry makes it possible to controllably carry out the modification of system components within a wide range. This work will present the results on the preparation of vinyl-containing polydimethylsiloxanes with controlled content of functional groups in the chain and molecular weight characteristics, by polycondensation of methylvinyldimethoxysilane and dimethidiethoxysilane in an active medium that is an excess of anhydrous acetic acid. The reaction scheme is shown in Figure 1. The paper investigated the effect of the ratio of the starting monomers, the temperature, and the duration of condensation of the obtained co-oligomers in a vacuum on the molecular weight characteristics of the product. The analysis of the products was carried out using a combination of physics and chemical research methods (NMR spectroscopy, GPC, GLC). The resulting vinyl-containing polymers appear to be a promising matrix for the preparation of polydimethylsiloxanes with polar groups.

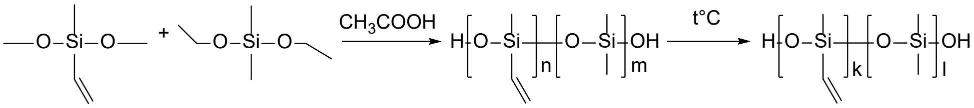


Figure 1. General scheme of the synthesis of functional copolymers

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

---

[1] Youn, Jung-Hwan, et al. *Applied Sciences* 2020, **10**(2), 640.

[2] M. D. Dickey, *Adv. Mater.*, 2017, **29**(27), 1606425

[3] Sheima, Yauhen, et al. *Macromolecules*. 2021.

[4] Perju, E., Shova, S., & Opris, D. M., *ACS applied materials & interfaces* 2020, **12**(20), 23432-23442.

Copolymers Based on Polyvinylidene Fluoride and Chlorotrifluoroethylene with Grafted Polyacrylonitrile or Poly (Ethyl Methacrylate) Chains for Ferroelectric Organic Field-Effect Transistors

E.A. Kleymyuk[1] *, *A.I. Nevelskaya*[1], *A.A. Trul*[1], *Yu.N. Luponosov*[1], *S.A. Ponomarenko*[1]

[1]Institute of Synthetic Polymer Materials RAS
*e-mail: kleymyuk@ispm.ru

The applications of fluoropolymers in electronic devices have been interested researchers for many years, especially because of their ferroelectric properties.[1,2,3,4,5] Polyvinylidene fluoride (PVDF) has a special position in this class of polymers, which shows piezo-, pyro- and ferroelectric properties, depending on the crystalline phase.[3] For example, for obtaining a polar crystalline phase β, required for ferroelectric properties, complex film processing methods are used, such as deformation, high-temperature annealing, and quenching techniques. To avoid possible difficulties, as well as to increase possible applications and adjust the properties, copolymers with grafted polar monomers can be used. In this work we report on novel copolymers based on PVDF and chlorotrifluoroethylene with grafted polyacrylonitrile (PAN) or poly(ethyl methacrylate) (PEMA) chains.[6] Using the controlled radical polymerization, we have synthesized polymers with various degree of PAN or PEMA grafting onto their side chains. The grafted chain content was determined by NMR spectroscopy. The effect of various synthetic parameters on the physical properties of the copolymers obtained is shown. The phase behavior and thermal stability of the samples were investigated by DSC and TGA methods.

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

---

[1] B. Ameduri, *Chem. Rev.*, 2009, **109**, 6632-6686.

[2] Chu, B. *Science*, 2006, **313**(5785), 334–336.

[3] X. Zhang, Ch. Zhang, Yu. Lin, P. Hu, Ya. Shen, K. Wang, S. Meng, Yu. Chai, X. Dai, X. Liu, Yu. Liu, X. Mo, C. Cao, S. Li, X. Deng, L. Chen, *ACS Nano*, 2016, **10**, 7279-7286.

[4] Z. Zhang, T. C. M. Chung, *Macromolecules*, 2007, **40**, 783-785.

[5] B. Stadlober, M. Zirkl, M. Irimia-Vladu, *Chem. Soc. Rev.*, 2019, **48**, 1787-1825.

[6] A. D. Khudyshkina, Yu. N. Luponosov, V. G. Shevchenko, S. A. Ponomarenko, *Express Polymer Letters*, 2021, **in print**

Origin of Poor Photovoltaic Performance of Bis(Tetracyanoantrathiophene) Non-Fullerene Acceptor

E.S. Kobeleva[1*], *A.A. Popova*[2], *D.S. Baranov*[1], *M.N. Uvarov*[1], *D.A. Nevostrueva*[1,2], *K.M. Degtyarenko*[3], *R.M. Gadirov*[3], *A.S. Sukhikh*[4], *L.V. Kulik*[1]

[1]Voevodsky Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Science
[2]Novosibirsk State University, Novosibirsk, Russian Federation
[3]Tomsk State University, Tomsk, Russian Federation
[4]Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academyof Sciences
*e-mail: gorgeouscleverowl@gmail.com

Previously, the prerequisites for the successful use of a new compound based on anthrathiophene 2,2 '- [2,2' - (5,5 '- (9,9-dioctyl-9H-fluorene-2,7-diyl) bis (ethyn- 2,1-diyl) bis (thien-5,2-diyl)) bis (11-oxo-anthra [2,1-b] thiophen-6-ylidene)] dimalononitrile (AT1) as a non-fullerene acceptor in a composite with a conjugated polymer PCDTBT for the production of photovoltaic cells were identified. However, the parameters of cells with anthrathiophenes turned out to be noticeably worse than those of cells based on a standard PCDTBT / PCBM composite. The methods of light-induced EPR and electron spin echo out of phase are used to determine the reasons for the low photovoltaic efficiency of AT1 in comparison with conventional fullerene acceptors. These methods showed that the average electron capture energy in PCDTBT / AT1 mixtures is higher than in PCDTBT mixtures with fullerene acceptors, while the initial photoinduced electron transfer is lower. It is assumed that these two effects increase the efficiency of geminal recombination of PCDTBT / AT1 mixtures, reduce the yield of free charges, which, as a limitation, is the main deterioration of photovoltaic parameters for mixtures, set AT1. Low electron mobility $\mu = 3.5 * 10^{-6}$ cm^{2}V^{-1}s^{-1} was estimated for AT1 from the photo-CELIV experiment. The strong localization of electrons on the terminal AT1 acceptor donors explains both the efficient geminal recombination in mixtures of an anthrathiophene-based acceptor with polymer donors and the low electron mobility in AT1.

This work was supported by RFBR (project № 20-33-70126).

Optical Properties of Selectively Fluorinated Furan-Phenylene Co-Oligomers

A. Kuimov[1], I. Koskin[1], C. Becker[1], A. Sonina[1], M. Kazantsev[1]*

[1]N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry SB RAS

*e-mail: anatoliikuimov@gmail.com

Highly emissive semiconductors are extremely valuable for light-emitting electronic devices. Nowadays a number of organic crystalline materials combining bright photoluminescence (PL) and semiconducting properties have been found.[1,2] Among them, furan-phenylene co-oligomers (FPCOs) having superior solubility, molecular rigidity and bright luminescence are considered to be promising.[3] Here we studied the optical properties of selectively fluorinated FPCOs based on 1,4-bis(5-phenylfuran-2-yl)benzene (FP5).

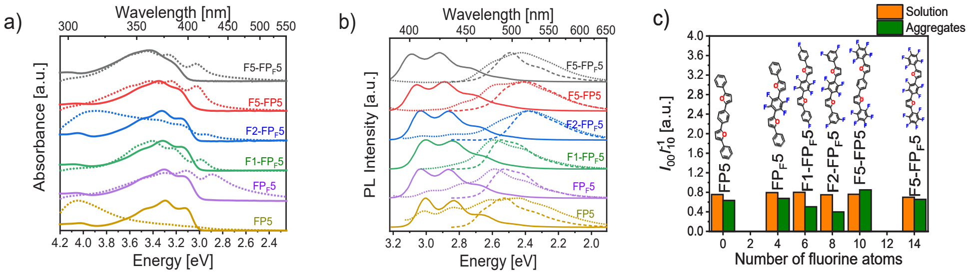


Figure 1. Optical absorption (a) and PL (b) spectra of FPCOs studied in THF (solid lines), binary mixtures THF:H_2O (aggregates, dotted lines) and single crystals (panel (b), dashed lines); ratio of 00 to 10 absorption peak intensities (c) for THF solutions, aggregates and the structures of the studied compounds.

Absorption spectra of fluorinated FPCOs (Figure 1a) demonstrated two representative trends: (i) the increase of fluorine atom number blue-shifts the absorption and emission maxima and (ii) the full fluorination of terminal phenyl groups causes a smoothing of the fine structure of the optical absorption spectrum which is associated with the decrease of molecular rigidity. All FPCOs demonstrated the H-aggregation behavior except F5-FP5 showing the signatures of J-aggregation. As all materials were synthesized by the cross-coupling reactions, self-dopants, arising as by-products, were found in all fluorinated FPCOs samples as earlier reported for FP5.[4] Fluorination of FP5 results in lower energies of frontier molecular orbitals and almost the same optical bandgap. All the FPCOs were highly emissive both in solutions with photoluminescence quantum yields (PL QY) of 80% and in crystals with PL QY of 47–60%. Selective fluorination is highlighted as powerful approach for the design of highly emissive organic semiconductor single crystals.

This work was supported by RSF (project № 20-73-10090).

---

[1] J. Gierschner, S. Y. Park, *J. Mater. Chem. C.* 2013, **1**, 5818

[2] H.-H. Fang, J. Yang, J. Feng, T. Yamao, S. Hotta, H.-B. Sun, *Laser Photonics Rev.* 2014, **8**, 687

[3] Kazantsev M. S. *et al.*, *Org. Electron.* 2018, **56**, 208-215

[4] Mannanov A. A. *et al.*, *J. Mater. Chem. C.* 2019, **7**, 60-68

Towards Understanding the Chemical Structure - Oxidation Stability Relationships for Conjugated Polymers Used in Organic Solar Cells

I.V. Martynov[1], L.N. Inasaridze[1], P.A. Troshin[1]*

[1]The Institute for Problems of Chemical Physics of the RAS,
*e-mail: martinov@mitht.org

The rapid development of the Internet of Things (IoT) technologies drives the massive implementation of portable electronic devices, wireless sensors, and self-powered electronics. Multiple devices integrated into IoT networks require very little power and often operate indoors. Organic photovoltaic (OPV) cells, which can harvest efficiently low-intensity indoor light, are ideal stand-alone power sources for such remote devices. Tremendous progress in organic photovoltaics resulted in certified power conversion efficiencies up to 18% for small-area devices. However, poor device stability represents the yet unsolved problem restricting the commercialization of this promising technology. Some fundamental relationships have to be established between the absorber materials' molecular structure and their stability to achieve sufficiently long operational lifetimes in organic photovoltaics. It is particularly important to understand the factors predefining the resistance of electron donor conjugated polymers to photooxidation since the manufacture and encapsulation of organic solar cells are carried out in the presence of oxygen under ambient conditions.

Here we addressed this challenge and systematically explored the photooxidation stability of a series of conjugated polymers comprising TBT and TTBTBTT monomer units (T - thiophene, B - benzothiadiazole) in combination with the building blocks X possessing different electronic and electrochemical characteristics. It has been shown previously that electron spin resonance (ESR) spectroscopy represents a highly sensitive technique to investigate the electronic quality and photostability of conjugated polymers.[1] The conjugated polymers form radical species under light and/or oxygen exposure.[2] Therefore, the stability of conjugated polymers can be assessed by analyzing the rates of the accumulation of radicals in their thin films as revealed by ESR spectroscopy.

In our experiments, the samples of conjugated polymers and their composites with [60]PCBM were annealed in air at 130 °C for 2 hours, which models the realistic solar cell encapsulation conditions. Afterward, the samples were sealed in the ESR glass tubes under an inert atmosphere and exposed to UV light. The ESR spectroscopy was used to reveal the rates of the accumulation of radical species, which were well correlated with the electrochemical oxidation potentials of conjugated polymers. It was shown that an increase in the material oxidation potential translates to improved photooxidation stability. Therefore, the most stable conjugated polymers comprise such building blocks as carbazole or fluorene. In contrast, the conjugated polymers incorporating electron-rich benzodithiophene and cyclopentadithiophene fragments were found to be the least stable. The established correlations between the molecular structures and properties of the conjugated polymers and their photochemical stability can guide the further rational design of highly stable organic absorber materials required for the practical implementation of organic photovoltaics.

The work was supported by the Russian Science Foundation (project 18-13-00205P). General support was also provided by the Ministry of Science and Higher Education of the Russian Federation within the project No. AAA-A19-119071190044-3 (0089-2019-0010)

---

[1] L.A. Frolova, N.P. Piven, D.K. Susarova, A. V. Akkuratov, S.D. Babenko, P.A. Troshin, *Chem. Commun.* 2015, **51**, 2242–2244.

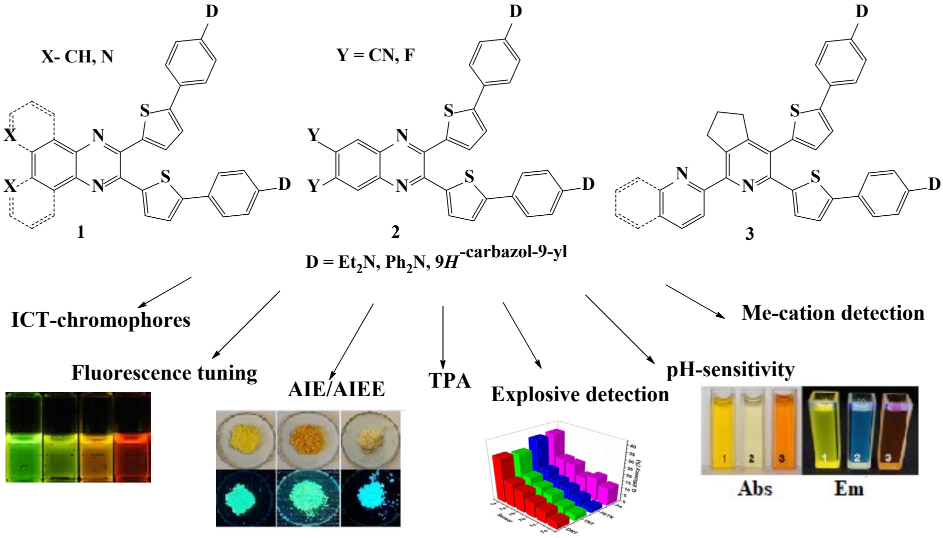
[2] L.N. Inasaridze, A.I. Shames, I. V. Martynov, B. Li, A. V. Mumyatov, D.K. Susarova, E.A. Katz, P.A. Troshin, *J. Mater. Chem. A.* 2017, **5**, 8044–8050.

P-17

V-Shaped Chromophores Based on Quinoxaline and Cyclopenta[*c*]Pyridine: Synthesis and Perspective Applications

T.N. Moshkina[1*], *A.E. Kopotilova*[1], *E.V. Nosova*[1,2], *G.N. Lipunova*[1,2], *V.N. Charushin*[1,2]
[1]Department of Organic and Biomolecular Chemistry Ural Federal University
[2]Postovsky Institute of Organic Synthesis Ural Division of the Russian Academy of Sciences
*e-mail: tan.moshckina@yandex.ru

Currently, interest is growing in V-shaped quinoxaline chromophores due to their potential applications in organic electronics.[1,2] 2,2'-Bipyridine derivatives served as chelating ligands in coordination chemistry and building blocks for the construction of efficient non-metal π-conjugated structures.[3]



A series of novel V-shaped 2,3-bis(5-arylthiophen-2-yl)quinoxalines and their dibenzo- and dipyrido- derivatives as well as counterparts containing fluorine atoms or CN-group at benzene ring have been designed and synthesized. Additionally, V-shaped cyclopenta[c]pyridine chromophores bearing pyridinyl or quinolinyl residue have also been obtained. The thienylquinoxaline chromophores, bearing diethylaminophenyl fragments, showed significant sensitivity towards the medium acidity with color changes and luminescence switching upon the introduction of acid.[4] Some of V-shaped derivatives **1** displayed fluorescence quenching upon addition of nitro-containing explosives; 2,3-bis(5-(4-diethylaminophenyl)thiophen-2-yl)-quinoxaline is the most representative chemosensor (K_{SV} = 48400–57800 M^{-1} and LOD = 32–216 ppb).[5] Two-photon absorption cross section of "green" chromophores of series **2** have found to reach 5900 GM. Cyclopenta[c]pyridine-contained chromophores **3** demonstrated bright luminescence in the solid state.

This work was supported by Russian Science Foundation (project № 19-73-10144).

---

[1] Gupta S., Milton M.D., *Dyes and Pigments*, 2019, **165**, 474–487.

[2] Ishi-i T., Moriyama Y., *Tetrahedron*, 2017, **73**, 1157–1164.

[3] Zhu L., Younes A.H., Yuan Z., et al., *J. Photochem. Photobiol. A Chem.*, 2015, **311**, 1–15.

[4] Moshkina T.N., Nosova E.V., et al, *Asian J. Org. Chem.* 2018, **7**, 1080–1084.

[5] Moshkina T.N., Nosova E.V., et al, *Asian J. Org. Chem.* 2020, **9**, 673–681.

A New Approach for Fabrication of Biorecognition Layer in Electrolyte-Gated Organic Field-Effect Transistors

E.Yu. Poimanova[1*], *P.A. Shaposhnik*[1,2], *V.P. Chekusova*[1], *D.S. Anisimov*[1], *A.A. Trul*[1],
M.S. Skorotetcky[1], *V.B. Krylov*[3], *E.G. Zavyalova*[2], *E.V. Agina*[1], *S.A. Ponomarenko*[1,2]

[1]Enikolopov Institute of Synthetic Polymeric Materials of RAS
[2]Chemistry Department of Lomonosov Moscow State University
[3]Zelinsky Institute of Organic Chemistry of RAS
*e-mail: poymanova@ispm.ru

Notwithstanding the evidence that organic field-effect transistors are rapidly emerging as ultrahigh sensitive label-free biosensors a call for high selectivity of electronic devices still remains[1]. A proof is needed that a given response is due only to the presence of the target analyte in a sample. There are different approaches for integration of biomolecules into the transistor device, they use modification of the surface of an active layer or the gate surface[2]. Here we present a new approach for fabrication of the biorecognition layer in electrolyte-gated organic field-effect transistors (EGOFET). It exploits the bi-layer structure (Fig. 1a) with receptors anchored to the organic semiconductor (OSC) surface. Flat crystals of an OSC active layer on SiO_2/Si wafer were obtained with Doctor Blade technique using blend of benzothieno[3,2-b][1]benzothiophene (BTBT) and polystyrene[3]. Bioreceptor layer was deposited by Langmuir-Schaefer technique using the blend of the organosilicon dimer of BTBT (D2-Hept-BTBT-Hex) with recently developed biotin containing derivative of this dimer. We tuned the proportion between the components of the blend from 100:1 to 1:1 to understand their mutual distribution on the surface. We controlled film formation by use of optical and atomic force microscopy. To prove the presence of biotin on the surface of bioreceptor layer fluorescent analysis and ELISA technique were used.

Electrical measurements in PBS as electrolyte in saturation (V_{DS}=-0.5 V) regime were conducted to measure transfer characteristics of the device with bioreceptor layer and after consistent immobilizations of streptavidin, biotinylated aptamer to hemagglutinin of influenza virus (RHA0385) and virus of influenza A (H5N1 strain, 10^9 virus particles per mL) or control virus (Newcastle Disease virus, 10^9 virus particles per mL) on the transistor channel. The positive shift in 0.1 V of threshold voltage was observed only in the case of influenza virus, the detection of which is based on the specific interaction of every immobilizied layer (Fig. 1b). We conclude that the presented technique of the biorecognition layer fabrication on the OSC surface is promising for the biosensing based on the biotin-streptavidin interaction.

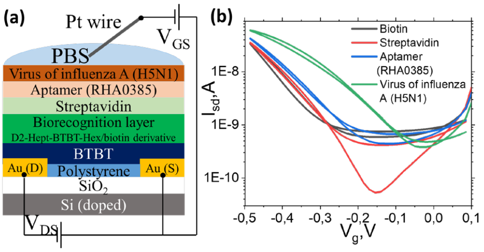


Figure 1 Scheme of fabricated device **(a)** and its EGOFET transfer characteristics **(b)**.

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

---

[1] Minamiki T. et al. *Commun. Mater.*, 2021, **2**, 1–8.
[2] Torsi L. et al. *Chem. Soc. Rev.*, 2013, **42**, 8612–8628
[3] Shaposhnik P.A. et al. *Dokl. Phys. Chem.*, 2021, **496**, 20–24.

P-19

Synthesis and Properties of New Organosilicon Derivatives of [1]Benzotieno[3,2-b][1] -Benzothiophene with Different Length of Terminal Aliphatic Substituents

M.S. Polinskaya[1*], *O.V. Borshchev*[1], *M.S. Skorotetcky*[1], *V.P. Chekusova*[1], *A.A. Trul*[1], *D.S. Anisimov*[1], *S.A. Ponomarenko*[1]

[1]Institute of Synthetic Polymer Materials RAS
*e-mail: polinskaya@ispm.ru

Currently, in organic electronics, much attention is paid to semiconductor materials based on [1]benzothiene[3,2-b][1]-benzothiophene (BTBT) due to their high mobility of charge carriers and stability of molecules[1]. The use of such compounds as functional materials using Langmuir technologies as a deposition method is one of the most promising, fast, and reproducible approaches for the manufacture of electronic devices[2]. The data obtained earlier allow us to conclude that the BTBT derivatives, which have an anchor siloxane group and an optimal length of an aliphatic spacer, have sufficiently high semiconductor characteristics when applying films by Langmuir methods[3]. However, the effect of terminal aliphatic substituents, which are introduced into the structure of the molecule to increase the solubility of the compound, on the semiconductor properties of the material has not been studied in detail. In this regard, the aim of this work was to synthesize and study the properties of organosilicon derivatives of BTBT with different lengths of terminal aliphatic substituents.

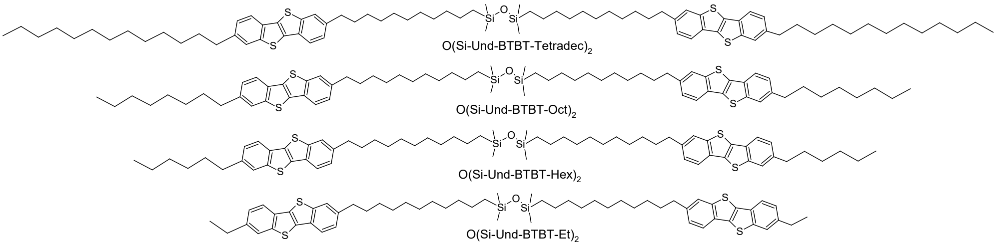


Fig. 1. Structural formulas of synthesized compounds.

The synthesis of the target compounds was carried out using a combination of successive Friedel-Crafts acylation reactions, keto group reduction, and hydrosilylation using a platinum catalyst. In accordance with the synthetic scheme, to protect the double bond on the undecylene spacer during the reduction of the keto group, it was previously protected by bromine atoms, which were removed immediately before the hydrosilylation reaction. All the final compounds were characterized by a complex of modern physical and chemical methods. The electrical properties of OFETs based on thin films made by Langmuir methods are studied. Their threshold voltages vary in the range from -3 to -9 V, and the values of the mobility of charge carriers lie in the range of 10^{-3}-10^{-2} cm^2 / Vs, which makes it possible to use such OFETs as gas sensors.

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

---

[1] Y. Yuan and all, *Nat. Commun.*, 2014, **5**, 3005.

[2] A. S. Sizov and all, *Langmuir*, 2014, **30,** 15327.

[3] A.A Trul and all, *Sensors and Actuators B: Chemical*, 2020, **321**, 128609.

Conductivity of Solution-Processed Thin Films of Chlorophyll Derivatives: Drop-Casting vs. Spin Coating

Yu.I. Sachkov[1,2*], *A.I. Koptyaev*[2], *V.V. Travkin*[1,2]

[1]Institute of Physics of Microstructures RAS
[2]Ivanovo State University of Chemistry and Technology
[*]e-mail: Sachkov@ipmras.ru

Recent studies show the potential of green materials, such as chlorophylls, for use in photovoltaic converters[1] and related fields, such as transistors, sensors *etc*[1]. However, there are still major drawbacks that impede successful incorporation of chlorophyll-like molecules in optoelectronic devices. Particularly, aggregation of molecules into superstructures of various shapes occur spontaneously, which noticeably affects their charge-transporting and optical properties. In this work, we studied the morphology and functionalities of thin films of methylpheophorbide *a* (hereinafter Pheo), a representative of a large class of tail-free analogs of natural chlorophyll. A comparison with metallated compounds, InCl-Chlorin e6 and InCl-pyroPheo recently synthesized in our lab, is also reported.

Since Pheo films cannot be obtained by thermal evaporation, the thin-film samples were obtained by two wet methods: spin-coating (S-films) and drop-casting (similar to inkjet printing, D-films). Concentrations and deposition conditions were selected in such a way as to provide the films with satisfactory structural quality and uniform thickness. Various practically important substrates were tested, including glass/ITO and ceramics with planar electrodes. X-ray diffractometry, white light interferometry, atomic force microscopy and optical spectroscopy were used for structural characterization; charge carrier mobility was extracted from two-terminal DC conductivity measurements, photocurrent was stimulated by a simulated sunlight.

S-films have a thickness of 40-80 nm and a mirror-smooth surface. The micropores with a depth almost equal to the film thickness and a width of 100 nm are randomly distributed on it (density about 3e6/mm^2). This complicates fabrication of sandwich-type devices and explains occurrence of electrical shorts through the Pheo layer. In contrast, D-films can only be obtained with thickness above 150 nm and are distinguished by rough surface and better molecular ordering within the grains. The D-films are noticeably more conductive than S-films, with thermal activation energy of conductivity about 0.6 eV (2.5 for S-films).

Similarly deposited films of InCl-complexes turned out to be more reliable for photoelectrical measurements because of the lower hysteresis and fast response to the applied potential (in case of Pheo, an ionic conduction should be hypothesized). Despite similar film morphology, the photocurrent is higher than in the Pheo films obtained and tested under the same conditions.

This work was supported by the RSF, project #20-13-00285.

---

[1] G.L. Pakhomov, V.V. Travkin, P.A. Stuzhin, O.I. Koifman. *RSC Advances.* 2021, **11**, 15131-15152

Lanthanide Complexes with 2-(Tosylamino)-Benzylidene-N-(Aryloyl)-Hydrazones in NIR OLEDs

D.S. Koshelev [1*], *A.D. Fedichkina* [1], *L.O. Tcelykh* [2], *T.Yu. Chikineva*[1], *V.V. Utochnikova*[2]
[1]Moscow State University, Faculty of Materials Science
[2]Moscow State University, Department of Chemistry
*e-mail: dan_kosh@mail.ru

Near-IR luminescence is currently attracting interest due to important technological applications in telecommunications and visualization. Ytterbium coordination compounds (CCs) are among the most promising NIR emitters because narrow emission bands. In our laboratory, it was found that the lanthanides CCs with 2-(tosylamino)-benzylidene-N-(**aryloyl**)-hydrazone demonstrate a high NIR luminescence QY (up to 1.4%), high absorption (up to 30000 $(M\cdot cm)^{-1}$), but low solubility, that results only in the one OLED emissive layer material demonstrated electroluminescent efficiency up to 50 µW/W.[1,2] To further optimize the properties of these compounds, we examined the effect of ligand halogenation on the solubility of these compounds (Figure 1a). Moreover, we studied the effect of the substitution by electron-donating and electron-acceptor fragments (Fig.1b) on the charge carrier mobility and, consequently, the OLED performance of the corresponding ytterbium with 2-(tosylamino)-benzylidene-N-(**aryloyl**)-hydrazones.

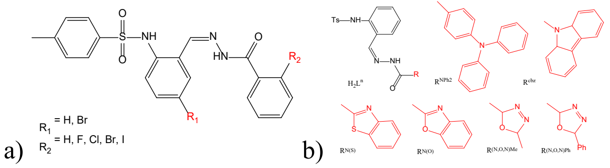


Figure 1. The structural formula of a) halogen-substituted b) aryloyl-substituted derivatives of 2-(tosylamino)-benzylidene-N-(**aryloyl**)-hydrazones ($H_2L^{\mathbf{R}}$).

The synthesis of the lanthanides CC was carried out by the reaction.

$$Ln(OH)_{3(ex)} + 2H_2L^{\mathbf{R}} \rightarrow Ln(L^{\mathbf{R}})(HL^{\mathbf{R}}) + 3H_2O \qquad (1)$$

$$Ln(L^{\mathbf{R}})(HL^{\mathbf{R}})_{(EtOH)} + KOH \rightarrow K[Ln(L^{\mathbf{R}})_2]_{(EtOH)} \qquad (2)$$

The composition of the obtained compounds was determined from a combination of data from ^1H, ^{13}C NMR spectroscopy, IR spectroscopy, TGA, and elemental analysis. It turned out that all halogen-substituted CCs, obtained by the reaction (1), possess solubility in THF, acetonitrile, and DMSO. It was also shown that the solubility increases with an increase in the number of halogen-substituents and with a decrease in their atomic mass. Thus, $Ln(^{\mathbf{Br}}L^{\mathbf{F}})(H^{\mathbf{Br}}L^{\mathbf{F}})$ shows the greatest solubility (up to 21 g/L in THF). NIR luminescence shows that the CCs QYs reach up to 1.9%. Testing of ytterbium complexes in OLED shows efficiency up to 140 µW/W for $Yb(^{\mathbf{Br}}L^{\mathbf{H}})(H^{\mathbf{Br}}L^{\mathbf{H}})$.

The lanthanide CCs with aryloyl-substituted ligands, obtained by reaction (1), possess a lower solubility than is required for use in OLED (5 g/L). The potassium salts of the CCs were obtained by reaction (2). Some of them achieved the required solubility. To obtain a host-free emissive layer the heteroleptic CCs based on the one electron-acceptor and one electron-donating ligand were obtained by two methods: a) complex mixing or b) ligand mixing. The Yb and Lu complexes composition in the solution was investigated by 1D and 2D NMR spectroscopy showing the presence of the heteroleptic CC. Testing of ytterbium complexes in OLED shows that the highest efficiency up to 120 µW/W was measured for heteroleptic CC $K[Yb(L^{\mathbf{NPh2}})(L^{\mathbf{(N,O,N)Ph}})]$. This electroluminescence spectrum at the same time demonstrates NIR emission for the most part.

This work was supported by RSF (project № 20-73-10053).

---

[1] Utochnikova, V. V. et al.. *Dalt. Trans.* 2015, **44**, 12660–12669.
[2] Kovalenko, A.D. et al. *Chem. Mater.* 2019*,* **31**, 759–773.

P-22

Europium β-Diketonates with Dipyrido [3,2-a:2′,3′-c] Phenazine in OLEDs

K.M. Kuznetsov[1*], *M.I. Kozlov*[1], *A.A. Vashchenko*[2], *V.V. Utochnikova*[3]

[1]Lomonosov Moscow State University, Department of Materials Science
[2]Lebedev Physical Institute of the Russian Academy of Sciences
[3]Lomonosov Moscow State University, Department of Chemistry
*e-mail: kirillkuz210801@gmail.com

One of the challenges in the development of organic light-emitting diode (OLED) technology is to improve color purity. It can be achieved by using coordination compounds of lanthanides as materials of the emission layers, since they have narrow luminescence bands (<10 nm). At the same time, lanthanide-based OLEDs have a rather low brightness, which is associated with the long lifetimes of the excited state. Among different classes of lanthanide coordination, compounds easily polarizable β-diketonates possess the lowest values of the lifeitimes. Hence, as the objects of study europium β-diketonates were chosen, which in addition are volatile and able to be deposited both by solution process and by vacuum thermal evaporation (VTE), while dipyrido [3,2-a:2′,3′-c] phenazine (DPPZ) was chosen as a neutral ligand, capable to quench the Eu^{3+} luminescence and thus also reduce the lifetime of excited state. Thus, the aim of this work is to obtain efficient solution-processed OLED based on europium β-diketonate with low lifetime of the excited state.

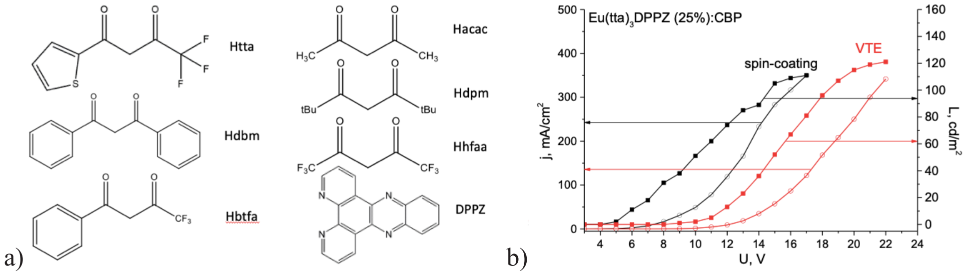


Figure 1. a) Ligands within the studied complexes, b) I-V and L-V curves of solution-processed and VTE-deposited OLEDs

The X-ray powder diffraction data coincided with the diffraction patterns calculated from the obtained single crystals of complexes $Eu(L)_3DPPZ$, where L = tta, dbm, btfa, acac, dpm, hfaa, which confirms the individuality of the synthesized compounds. The composition of $Eu(L)_3DPPZ$ (L = tta, dpm, btfa, acac, dbm, hfaa) complexes was established from the thermal analysis and ^1H NMR spectroscopy data.

According to photoluminescence data, all the complexes have rather low quantum yields (~1%), except for $Eu(btfa)_3DPPZ$ with PLQY = 23%. Also, the obtained complexes have short lifetimes of the excited state, which makes them promising for testing in OLEDs. For that, we chose $Eu(tta)_3DPPZ$, whose quantum yield to lifetime ratio is the largest among these complexes.

A series of diodes with a heterostructure ITO/PEDOT:PSS/poly-TPD/ $Eu(tta)_3DPPZ$ (25 wt%):CBP/TPBi/LiF/Al was manufactured, in which an emission layer was deposited by both spin-coating and VTE. The maximum brightness of $Eu(tta)_3DPPZ$ electroluminescence deposited from the solution was 111 cd/m^2 at 17 V, whereas the maximum brightness of a similar OLED, the emission layer of which was obtained by co-deposition in a vacuum, reached 121 cd/m^2 at 22 V. So, while their performance was similar, operating voltage of the solution-processed diode was 5 V lower than that of the VTE-deposited diode at the same brightness and current densities, which speaks in favour of the solution technology superiority. We demonstrated that it was a result of the higher density of the spin-coated emission layer.

P-23

Organic Electronic and the Opbital Properties Singlets, Triplets, Duplets, Quartets Electronic Excited States in the Series Multiatomic Compounds of Fluorescence and Generation of Dye-Lasers

A.E. Obukhov[1]*

[1]FAE “25th State research Institute of chemmotology of the Ministry of defense of Russia”
*e-mail: aobukhov@fo.gpi.ru

The spectral properties of understand and mechanisms of spin recombination reactions in the ground electronic state (*GrElSt*) and under the conditions of the kinetics of formation at deactivation of the electron-vibrational excitation energy (for the multistage of ionizations, dissociations, fragmentations, ion-radical recombinations, and detonation combustion) at desactivations in the full spectra of the electronic singlet and triplet (doublet and quartet for ion radicals) excited states to the scheme[1]:

$$S_0 \to h\nu_{exit,1} \to S_i^* <\approx> T_f^{\alpha} \approx> T_1 \to h\nu_{exit,2} \to T_j \approx I^* \approx> D_0^+ + e^-(\Delta E^*_{vibr})\cdot$$

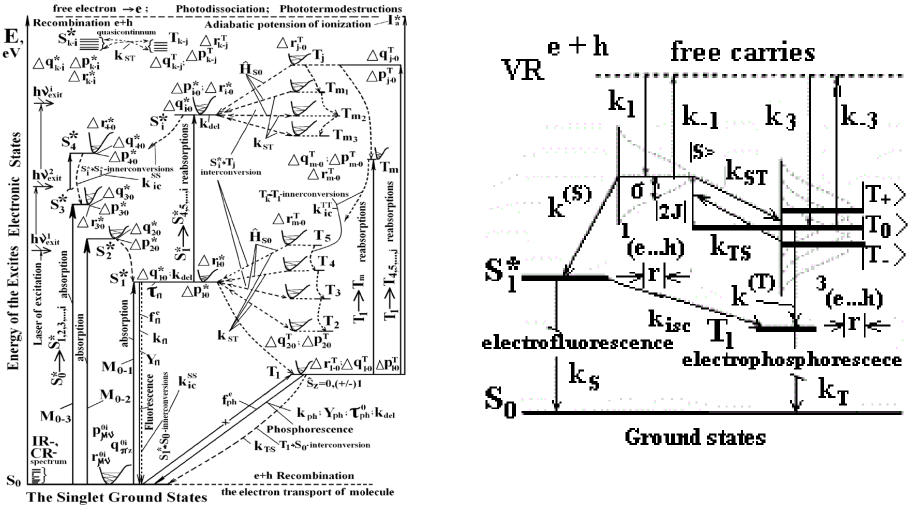

(a) (b)

Figure 1. The multilevels systems of radiative (fluorescence and phosphorescence) and non-radiative (of intercombination (InCC)) and electron-vibrational of internal conversions (InC)) on the multi-stage transitions in full the spectrum of singlet and triplet (S^*_i, T_j) electronically excited states $S^*_iT_jD^*_nQ^*_m ElExSt$ (D^*_n - doublet and Q^*_m - quartet forf ion) ("elementary act”) for polyatomic compounds, calculated by LCAO-MO SCF extended-CI INDO/S. When reionization (*I***) by secondary of electrons in the spectra $S^*_iT_jD^*_nQ^*_m ElExSt$ in plasma has been observed chemiluminescence of radicals: -$^\bullet$OH,-CHO$^\bullet$,-$_2$H=C-O$^\bullet$. (b) The energy-scheme of radiative (chemiluminescence) and non-radiative transitions in multiatomic compounds of resulting from bimolecular recombination (BMR), which are formed by the rate constants (k_1, k_{-1}, k_3, k_{-3}, $k^{(s)}$ and $k^{(T)}$.
1

---

[1] Obukhov, A.E. *Laser Physics*, 1997. **7**(5), 1102-1131.

P-24

Rejuvenation of Two-Phase Composite Employing Liquid-Gas Phase Transition Using Different Solvents

I.V. Bezsudnov[1*], *A.A. Kalinina*[1], *A.G. Khmelnitskaya*[1], *E.V. Agina*[1], *S.A. Ponomarenko*[1,3]
[1]Enikolopov Institute of Synthetic Polymeric Materials of RAS
*e-mail: bezsudnov_iv@ispm.ru

Two-phase composite material showing high volume expansion with rising temperature based on phase liquid-gas phase transition was initially invented in[1]. To prepare the composite the ethanol is added to component(s) of silicone compound. During the curing of the prepared mixture, the component that holds ethanol is consumed resulting in second phase formation in the forms of pores in silicone matrix initially filled by ethanol. Heating such a composite over boiling temperature of ethanol leads to its liquid-gas transition and accordingly to the high-volume composite expansion.

The volume expansion measurement device PARUS used in cycling mode allows us to measure composite in air. For all investigated composites we found that only four-five noticeable air cycles are possible, see Fig.1*a,b*.

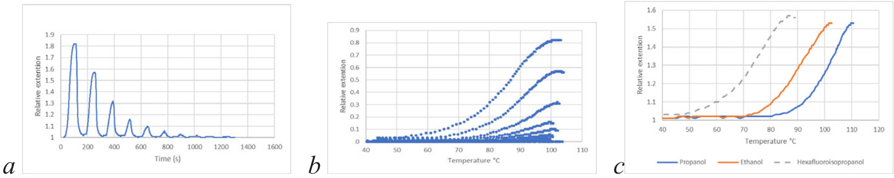


Fig1. Composite prepared with 15% ethanol, testing in cycling mode, a) relative extension vs. time, b) relative extension vs. temperature during heating phase, c) composite rejuvenated in ethanol (78°C), propanol (97°C), and hexafluoroisopropanol (58°C), first heating cycle.

The procedure of rehabilitation of the composite in[2] was named rejuvenation. The used composite was immersed back to ethanol for a day, new tests gave results as if the composite was in initial state. Our experiments show the same rejuvenation result even the composite sample was put only in ethanol vapors.

Also, we extended rejuvenation procedure using different solvents. We used propanol, isopropanol and hexafluoroisopropanol. In all cases, the procedure was successful. Actual properties of composite are changed accordingly to boiling temperature of used solvent. Fig.1c shows the silicone composite but rejuvenated with different solvents.

Therefore, we found the modification of rejuvenation procedure that results in great possibility to govern two-phase silicone composite properties even the manufacturing procedure remains unchanged i.e., using ethanol. Also, such two-phase composite demonstrates a very seldom possibility when one of the phases can be fully exchanged to another substance (solvent).

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

---

[1] A.Miriyev, K.Stack, H.Lipson, *Nat. Commun*. 2017, **8**.

[2] A.Miriyev, C.Trujillo, G.Caires, H.Lipson, *MRS Commun*., doi:10.1557/mrc.2018.30

P-25

Fabrication of the Patterned Polymer Substrates for Fully Printed Polymer OFET Creation

V.P. Chekusova[1*], *A.A. Trul, E.V. Agina*[1]

[1]Institute of Synthetic Polymer Materials RAS
*e-mail: chekusova@ispm.ru

Using of printing technologies is simple, ecological and safe approach allowing to fabricate easy scalable cheap sensors with wide range of applications. Transition from traditional silicon substrates to printed polymer ones supposed to avoid a lot of difficulties associated with device fabrication as well as to create flexible and/or stretchable sensors.

The main task of our work was to develop a reliable technique to fabrication of fully printed polymer field-effect transistor (PPFET) for gas sensing. To achieve this goal it is necessary to elaborate suitable PPFET architecture and a method of sequential printing of additive layers such as electrodes, interface, dielectric, semiconductor on polymer substrate.

All devices were fabricated on glass or polyethylene naphthalate (PEN) substrates in bottom contact – bottom gate geometry (Fig.1a). In order to provide sufficient adhesive properties of silver (Ag) inks to substrate, the substrate surface has been treated by oligomeric 3-aminopropyltriethoxysilane using spin-coating[1]. The bottom gate was printed by two ways: screen and inkjet printing. To ensure compatibility with the previously elaborated electronics required to sensory properties measurement, the same pattern of electrodes configuration was used.[2] For inkjet printing conditions such as pulse shape, firing frequency, piezo voltage, meniscus pressure and permission were selected and optimised. Commercial silver inks were used for printing. To provide contact layer stability post-treatment annealing was carried out at 150 degrees in a vacuum oven. It should be notice that annealing at a lower temperature or without vacuum doesn't provide the required layer stability, which leads to the damage of the electrodes during a dielectric layer formation. The dielectric layer was deposed by Dr. Blade technique as a kind of screen printing. The dielectric layers fabrication conditions such as molecular weight (MW) of polystyrene (PS), PS concentration and solvent composition were optimized. The dielectric layer quality was estimated by AFM morphology, layer capacitance and density of leakage current. The best characteristics of layer (RMS = 0.26nm, specific capacitance = 27 nF/cm^2) were achieved for the device fabricated on glass substrate with inkjet printed electrodes and dielectric layer obtained from toluene (90%)/o-xylene (10%) solution of PS with MW= 280k g/mol at concentration of 60 mg/ml.

Obtained characteristics allow to concluded that fabricated printed substrates should be suitable for further PPFET fabrication.

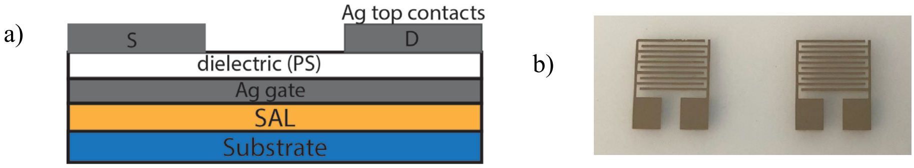


Fig. 1. Schematic representation of selected PPFET's architecture (a) and photo of the screen-printed source and drain electrods (b).

This work was supported by RFBR (project № 20-33-90236).

---

[1] M.N. Kirikova, et.al, *J.Mater. Chem. C.*, 2016, **4(11)**, 2211–2218

[2] A.A. Trul, V.P. Chekusova, et.al, *Sensors and Actuators B: Chemical*, 2020, **321**, 128609

P-26

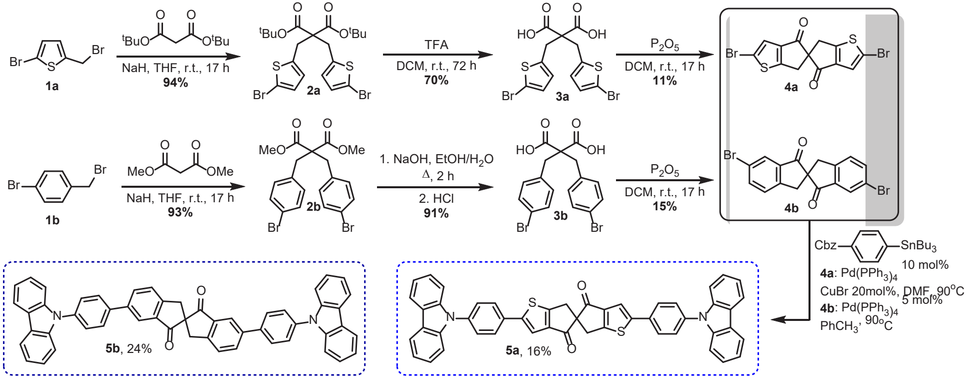
Carbazole-Decorated Spiroconjugated Pure Organic Phosphorescent Materials Based on 2,2'-Spirobi[indene] and 5,5'-Spirobi[cyclopenta[b]thiophene] Linkers

D.E. Samburskiy[1*], *K.S. Ivanov*[1], *R.Yu. Peshkov*[1], *E.A. Mostovich*[1]
[1]Novosibirsk State University
*e-mail: d.samburskii@g.nsu.ru

Development of pure organic phosphorescent emitters, which possess long-lasting, yet efficient phosphorescence at room temperature, appears to draw a lot of attention since it has a wide range of applications in organic light-emitting diodes (OLEDs), bioimaging, and encryption technologies.

Fundamental principles of constructing such materials are (1) enhancing of the intersystem crossing rate constant (k_{ISC}), which can be achieved through diminishing energy gap (ΔE_{ST}) between S_1 and T_1 excited states; (2) enhancing of the emissive transition rate ($T_1 \rightarrow S_0$) via introduction of heteroatoms (O, N, S, P, etc.); (3) minimizing the contribution of the non-radiative energy losses and triplet state quenching processes through the molecular rigidification.

Herein we developed an approach to carbazole-decorated highly rigid 2,2'-spirobi[indene] and 5,5'-spirobi[cyclopenta[*b*]thiophene] and investigated their optoelectronic properties.



The syntheses include the sequential alkylation of malonic ester with the corresponding bromides **1a**,**b**, hydrolysis of the obtained esters **2a**,**b** and intramolecular spirocyclization of the resulting acids **3a**,**b** in the presence of P_2O_5. In case of spiro-compound **4b** the final stage implies the application of the standard Stille cross-coupling protocol. However, in case of **4a** the modified Stille cross-coupling reaction was used, which features CuBr additive. Optical and electronic properties of **4a**,**b** were investigated using UV-Vis, fluorescent spectroscopy, and cyclic voltammetry. TD DFT calculations were used for theoretical study of geometry, frontier orbitals, ground and excited states.

As a result, it was demonstrated that 2,2'-spirobi[indene] and 5,5'-spirobi[cyclopenta[*b*]thiophene] structural motives provide with a variety of structural modifications that can be utilized for designing pure organic phosphorescent materials.

This work was supported by Russian Science Foundation (project № 19-13-00327) and Ministry of Science and Higher Education of Russian Federation project No FSUS-2020-0036

P-27

Physical Modeling of the Charge and Excitation Transport in QD-Based and Hybrid Photovoltaic Cells

A.Yu. Saunina[1*], *V.R. Nikitenko*[1], *A.A. Chistyakov*[1], *M.A. Zvaigzne*[1], *A.R. Tameev*[2], *A.E. Aleksandrov*[2]

[1]National Research Nuclear University "MEPhI" (Moscow Engineering Physics Institute)
[2] A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS
*e-mail: ayus03@mail.ru

In photovoltaic cells based on PbS colloidal quantum dot (CQD) solids, the photoconductivity and efficiency for PbS CQDs with inorganic atomic ligands of tetrabutylammonium iodide (TBAI) are reasonably larger than those for PbS CQDs with molecular ligands of the same length. The TBAI ligands can act as electron-transporting sites and contribute to the increase in mobility[1]. The basic Shockley-Queisser model[2] for the calculation of the power conversion efficiency does not take into account characteristics of the charge carriers and exciton transport, and thus, could not provide the deeper understanding of the effects of such characteristics on the cell perfomance.

The developed simple model includes drift and diffusion of electrons and holes, as well as diffusion of excitons and allows the maximum efficiency of a CQD solar cell to be determined, which can be achieved by eliminating the recombination losses of charge carriers. The model offers the analytical expression for the J-V characteristics, which includes the effective parameters, such as exciton diffusion length, exciton boundary conditions and charge mobilities. Both experimental data and theoretical modeling testify in favor of the hopping nature of the electron transport in CQD–solids[3].

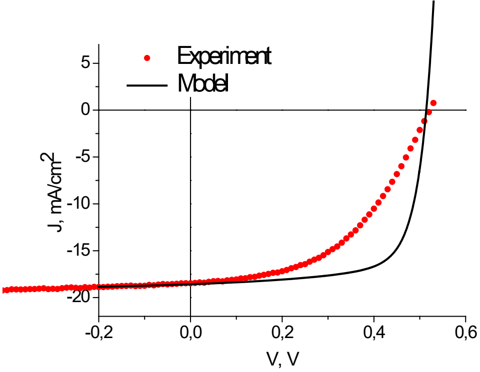


Figure 1. Experimental (symbols) and calculated according to the presented model (solid line) J-V characteristics of a QD-based solar cell.

Figure 1 illustrates the experimental and calculated J-V characteristics for ITO/PEDOT:PSS/PbS_{TBAI}/ZnO/Al cell based on 2.9 nm PbS QDs with TBAI ligands. The power conversion efficiency of 4.7% and 6.8% obtained from the experiment and simulation, respectively, shows that the charge recombination processes lead to the 31% power loss, which is reflected in the decreased fill factor.

---

[1] Stavrinadis A. *et al., Acs Energy Letters* 2017, **2**, 739–74410.

[2] Shockley W., Queisser H.J., *J. Appl. Phys.* 1961, **32**, 510.

[3] Saunina A.Y. *et al., J. Phys. Chem. C* 2021**, 125**(11), 6020-6025.

P-28

Method for Estimating the Photoluminescence Quantum Yield of Extremely Thin Organic Crystals

V.G. Konstantinov[1,2*], *A.I. Dorokhov*[1], *D.Yu. Paraschuk*[1,2]

[1]Moscow State University, Department of Physics
[2]Institute of Synthetic Polymer Materials RAS
*e-mail: vg.konstantinov@physics.msu.ru

Photoluminescence (PL) quantum yield (QY) measurements, required for selecting effective light-emitting materials, are usually provided by integrating sphere technique[1]. The integrating sphere technique is well suited for bulk samples, but it is hardly suitable for extremely thin (down to one molecular layer thick) samples with lateral sizes about 100 um due to low PL arriving from one or a few molecular layers collected from small lateral area.

In this contribution, we suggest a method for estimating the PL QY of extremely thin organic crystals – 2D single crystals of thiophene-phenylene co-oligomers – by using a combination of confocal PL microscopy for PL measurements and photothermal deflection technique for absorption measurements. Comparing absorption and PL intensity of the sample under study with those for a reference sample with known PL QY (solid solution of organic dye molecules in paraloid matrix) and assuming their PL directional diagrams, we obtain the PL QY of the former one. The details of the experimental techniques will be presented and discussed.

This work was supported by RSF (project № 18-12-00499).

---

[1] de Mello J.C., Wittmann H.F., Friend R.H. *Advanced Materials* 1997, **9**(3), 230–232.

P-29

Role of the Reorganization Energy for Charge Transport in Disordered Semiconductors

R. Saxena[1*], *V. R. Nikitenko*[2], *I. I. Fishchuk*[3,4], *Ya. V. Burdakov*[2], *Yu. V. Metel*[2], *J. Genoe*[5],
H. Bässler[6], *A. Köhler*,[1,6], *A. Kadashchuk*[4,5]

[1] Soft Matter Optoelectronics and Bavarian Polymer Institute (BPS), University of Bayreuth
[2] National Research Nuclear University “MEPhI” (Moscow Engineering Physics Institute)
[3] Institute for Nuclear Research, National Academy of Sci. of Ukraine
[4] Institute of Physics, National Academy of Sciences of Ukraine
[5] Interuniversity Microelectronics Centre (IMEC)
[6] Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth
*e-mail: rishabh.saxena@uni-bayreuth.de

While it is commonly accepted that the activation energy of the thermally activated polaron hopping transport in disordered organic semiconductors can be decoupled into a disorder and a polaron contribution, their relative weight is still controversial. This feature is quantified in terms of the so-called C-factor in the expression for the effective polaron mobility: $\mu_e \propto exp[-E_a/k_BT - C(\sigma/k_BT)^2]$, where E_a and σ are the polaron activation energy and the energy width of a Gaussian density-of-states (DOS), respectively. A key issue is whether the universal scaling relation (implying a constant C-factor) regarding the polaron formation energy is really obeyed in the same disordered system, as recently claimed in literature.[1] In the present work, we reinvestigate this issue on the basis of the Marcus transition rate model using extensive kinetic Monte Carlo simulations as a benchmark tool. We compare the polaron-transport simulation data with results of analytical calculations by the effective medium approximation (EMA) and multiple trapping and release (MTR) approaches. The key result of this study is that the C-factor for Marcus polaron hopping depends on first whether quasiequilibrium has indeed been reached, further on the σ/E_a ratio (Figure 1a), and finally on the degree of carrier localization, i.e., the coupling between the sites (Figure 1b). This implies that there is no universal scaling with respect to the relative contribution of polaron and disorder effect. Finally, we demonstrate that virtually the same values of the disorder parameter σ are determined from available experimental data using the C-factors obtained irrespective to whether the data are interpreted in terms of Marcus or Miller-Abrahams rates. This implies that molecular reorganization contributes only weakly to charge transport, and it justifies the use of the zero-order Miller-Abrahams rate model for evaluating the DOS width from temperature dependent charge transport measurements.

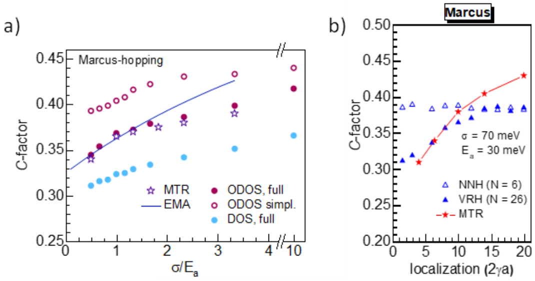


Fig. 1. C-factor vs. a) σ/E_a ratio ($2\gamma a = 10$) and b) localization parameter derived using Marcus rate in an isotropic 3D system. “DOS, full” refers to the case of non-equilibrated transport, all other data is obtained for transport under equilibrium.

---

[1] K. Seki and M. Wojcik, *J. Chem. Phys.* 2016, **145**, 034106.

A Study on the Stability of Electrolyte-Gated Transistor Based on 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene Blends with Polystyrene

P.A. Shaposhnik[1,2]*, *E.Yu. Poimanova*[1], *D.S. Anisimov*[1], *A.A. Trul*[1], *E.V. Agina*[1], *S.A. Ponomarenko*[1,2]

[1]Enikolopov Institute of Synthetic Polymer Materials RAS
[2]Lomonosov Moscow State University, Department of Chemistry
*e-mail: polinashaposhnik@ispm.ru

Point-of-care devices are booming branch of modern medicine industry as it enables available and precise medical diagnostics. One of the most promising platforms for such devices is electrolyte-gated organic transistors (EGOT). EGOT-based biosensors show ultra-low detection limits for various biomarkers. However, they encounter some problems with the baseline stability of parameters that serve as an analytical signal for this type of sensors (threshold voltage, maximum of source-drain current, transconductance). The decrease of these parameters could be attributed both to the influence of the electrolyte composition change (introduction of an analyte) and to the deterioration of the device performance. Therefore, study of EGOTs behavior during electrical measurements and storage is important for defining optimal operation mode and time limits of the device reliability. In this work, we focused on the long-term stability of EGOT based on 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene (C8-BTBT) blends with polystyrene reported recently from our laboratory[1].

We aimed to investigate how the electrical measurement parameters can influence stability of the EGOT during continuous cyclic measurements. At least two factors can negatively affect the device electrical characteristics: bias stress conditions and contact with electrolyte. The first factor is mostly associated with charge traps in the semiconductor/electrolyte interface and can be tuned with proper electrical measurement parameters. That means the electrical measurement protocol should include recovery time after each voltage application point. On the contrary, the decrease of device electrical performance due to a contact with electrolyte arises due to semiconductor material degradation and measurement time increase should not improve the device stability. We compared transfer characteristics measured with and without the recovery time (0.5 s) between the voltage application steps. In the case of the recovery time usage, we observed slower current decreasing and threshold voltage increasing. This indicates that electrical performance deterioration may be attributed to the charge trapping during the experiment rather than to the material degradation.

To estimate the shelf life of the devices in various conditions we measured transfer characteristics of the EGOT once a day for two weeks. We used deionized water for one group of devices and phosphate buffer saline (PBS) for another group to estimate the influence of electrolyte strength on the device stability. The third group was tested with water on the first day of the experiment and then was kept under reduced pressure without exposing to electrolyte. For devices measured in water, PBS, source-drain current (I_{SD}) decreased by an order of magnitude after ten days of the measurements, but nevertheless I_{SD} was higher than 1×10^{-7}A. Surprisingly, after two weeks we had not found any significant difference between all three groups of EGOT: all the devices showed a low current of about 50 nA. Atomic force microscopy showed increasing in surface roughness for all the devices. Therefore, the storage conditions are not crucial for the long-term stability of devices based on C8-BTBT blends with polystyrene.

This work was financially supported by a grant from the RSF (No. 19-73-30028).

---

[1] Shaposhnik P.A. et al. *Doklady Physical Chemistry*. 2021, **496**(2), 20–24.

P-31

Charge Transport in Single Crystals of 1,4-Bis(5-phenylfuran-2-yl)Benzene and its Fluorinated Derivatives

N.A. Shumilov[1,2*], *M.S. Kazantsev*[1]

[1]N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry SB RAS
[2]Novosibirsk State University
*e-mail: nikitashumilov1998@gmail.com

Nowadays, materials design is one of the most efficient ways in the development of organic optoelectronics. To achieve the best characteristics of organic devices it is indispensable to study fundamental "structure-property" relationships. Furan-phenylene co-oligomers (FPCOs)[1] are among the most intriguing emissive semiconductors due to their inherent combination of high charge mobility, luminescence, molecular rigidity and solubility. The introduction of substituents e.g. fluorine atoms is one of the most efficient approach for the tuning of crystal structure and optoelectronic performance of liner conjugated small molecules.

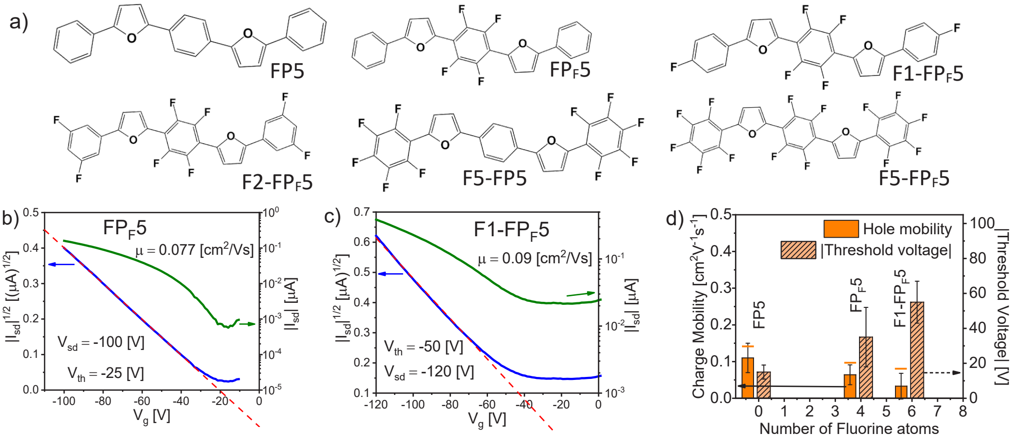


Fig. 1. The structures of investigated compounds (a). Transfer (saturation regime) characteristics of top-contact top-gate OFETs with FP$_F$5 (b) and F1-FP$_F$5 (c) single crystal OFETs. Maximal (horizontal bars) and average mobilities and threshold voltages of single crystal OFETs (d).

Here we studied the charge transport in single crystals of 1,4-bis(5-phenylfuran-2-yl)benzene (FP5) and FPCOs with fully/partially fluorinated central or edge phenyl rings (Fig. 1a). Top-contact top-gate OFETs with graphite-painted electrodes and parylene N gate dielectric were fabricated. The hole mobility of 0.12 cm^2/Vs and threshold voltage of -15 V were measured for FP5 in the saturation regime. Contrary, the performance of fluorinated FPCOs' single crystals are lower (Fig. 1b, c, d), heavily fluorinated F2-, F5-FP$_F$5, and F5-FP5 demonstrating no field-effect. The decrease of mobility and increase of threshold voltage for selectively fluorinated FPCOs is associated with the deterioration of hole injection because of (i) lowering of HOMO/LUMO energies and (ii) the surface-dipole effect of strong electron-withdrawing substituents (fluorine atoms). We conclude, that selective fluorination is efficient strategy of retaining efficient hole transport and inducing the electron transport in FPCO single crystals.

This work was supported by RSF (project № 20-73-10090).

---

[1] Kazantsev M.S. et al., *RSC Adv.*, 2016, **6**, 92325-92329.

P-32

Triphenylamine-Based Small Molecules for Pixelated Full-Colour Semiconductor Devices Towards Artificial Retinas

A.N. Solodukhin[1]*, D.O. Balakirev*[1]*, N.K. Kalinichenko*[1]*, P. Giannakou*[2]*, M. Shkunov*[2]*,*
Yu.N. Luponosov[1]*, S.A. Ponomarenko*[1]

[1] Enikolopov Institute of Synthetic Polymeric Materials RAS
[2] Electrical and Electronic Engineering, Advanced Technology Institute, University of Surrey
*e-mail: solodukhin@ispm.ru

Opto-stimulation of semiconductor-biointerfaces provides efficient pathways towards eliciting neural activity through selective spectral excitation.[1] In visual prosthesis, tri-colour excitation capability is the key to restoring full-colour vision. Here we report on investigation of organic photoactive π-conjugated donor-acceptor small molecules based on triphenylamine whose absorption spectra are similar to those of the photoreceptors of the human eye (Fig. 1).[2]

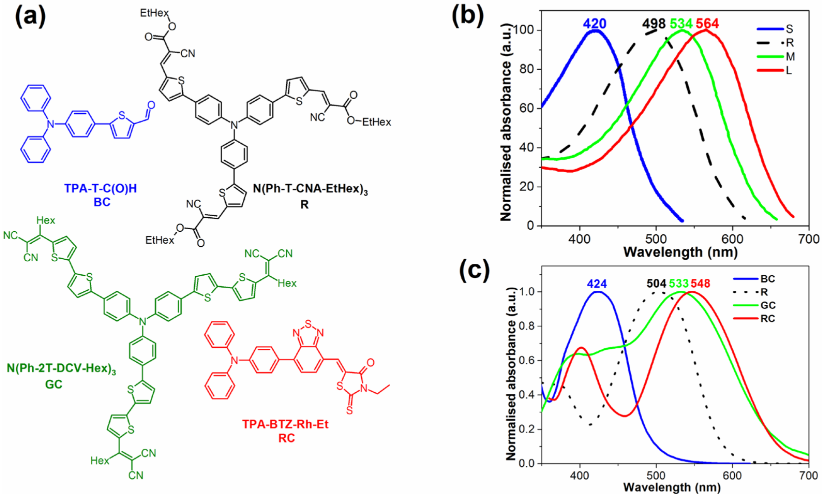


Fig. 1. (a) chemical structures of D-A molecules (b) spectral absorption curves of the short (S), medium (M) and long (L) wavelength pigments in human cones and rod (R) cells (c) normalised absorption spectra of thin films on glass of D-A molecules

Photoactive device fabrication and characterization towards full colour, pixelated retinal prosthesis based on inkjet printing of these molecules is demonstrated, with round pixels reaching 25 microns in diameter. Photo-response is studied via interfacing with biological electrolyte solution and using long-pulse, narrow-band excitations. Both photo-voltage and photo-current responses show clear signatures of capacitive charging at the electrolyte/device interface, also demonstrating spectral selectivity comparable to that of human eye’ cones and rods.

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

---

[1] Maya-Vetencourt J.F., Ghezzi D., Antognazza M.R., Colombo E., Mete M., Feyen P., Desii A., Buschiazzo A., Di Paolo M., Di Marco S., Ticconi F., Emionite L., Shma D.l, Marini C., Donelli I., Freddi G., Maccarone R., Bisti S., Sambuceti, G. Pertile G., Lanzani G., Benfenati F., *Nat. Mater.*, 2017, **16**, 681–689.

[2] Skhunov M., Solodukhin A.N., Giannakou P., Askew L., Luponosov Yu.N., Balakirev D.O., Kalinichenko N.K., Marko I.P., Sweeney S.J., Ponomarenko S.A. *J. Mater. Chem. C* 2021, **9**, 5858-5867.

P-33

Crystal Structure of Selectively Fluorinated Furan-Phenylene Co-Oligomers

A.A. Sonina[1*], *A.D. Kuimov*[1], *I.K. Shundrina*[1], *M.S. Kazantsev*[1]

[1]N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry of SB RAS
*e-mail: belalina04@gmail.com

Furan-phenylene co-oligomers (FPCOs) are promising materials for organic optoelectronics due to superior solubility (compared to their thiophene analogues), high photoluminescence quantum yields and charge mobility[1]. However, the systematic study of their substituted derivatives, in particular with electron-withdrawing groups is still lacking[2].

In this work a series (Fig. 1) of 1,4-bis(5-phenylfuran-2-yl)benzene (FP5) derivatives with high luminescence efficiency were crystallized and studied. All fluorinated FPCOs possess a face-to-face π-stacking arrangement (Fig. 1) contrary to the herringbone motif of unsubstituted FP5[1]. Since phenyl fluorination causes a deficit of the electron density at the center of this ring, the phenyls in π-π stacks are aligned with the furans with a lateral displacement (x- and y- slips, Fig. 1). The direction of π-π-stacking corresponds to the direction of crystal growth for elongated-shaped crystals. Molecules in F5-FP5 and F2-FP$_F$5 crystals exhibit nearly perpendicular orientations of the long molecular axes in respect to the main crystal facet (δ_T), whereas FP$_F$5, F1-FP$_F$5 and F5-FP$_F$5 demonstrate a remarkable inclination. According to our intermolecular interaction analysis in all fluorinated FP5s molecular π-stacks are stabilized by C-F··· π interactions, are connected by intralayer and interlayer C-H···F interactions and interlayer F···F close contacts (terminal fluorinated FP5s) and C-H···π interactions for FP$_F$5.

Upon the fluorination of central phenylene ring (FP$_F$5) the solubility in toluene increases and fluorination of the terminal phenyl ring decreases the solubility. According to the DSC analysis the melting points exhibit a mirror trends: a decrease/increase upon fluorination of the phenylene/phenyl moiety.

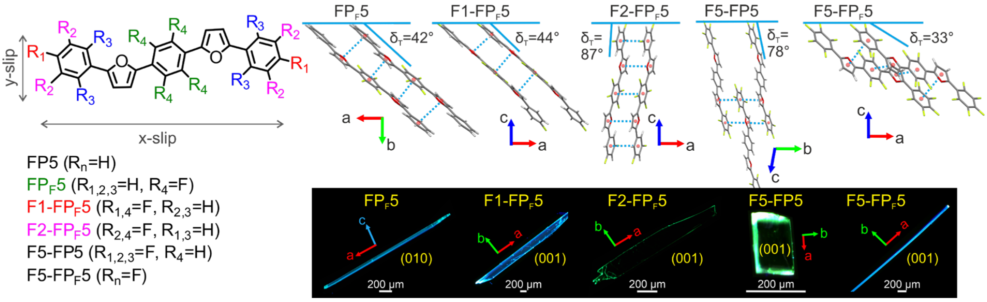


Fig. 1. The chemical structure, fragments of crystal structures in respect to the main crystal facet and single crystals under blue laser irradiation (405 nm) of fluorintated FPCOs.

In summary, we have demonstrated a series of highly-emissive single crystals based on fluorine-substituted furan-phenylenes. The crystal packing, intermolecular interactions solubility and thermal stability of linear conjugated oligomers can be effectively tuned by the selective introduction of fluorine substituents.

This work was supported by RSF (project № 20-73-10090).

---

[1] Kazantsev M.S. et al. *RSC Adv*. 2016, **6**(95), 92325-92329.

[2] Sonina A.A. et al. *Acta Cryst. B*. 2018, **75**(5), 450-457.

P-34

Charge Transport Highways Within Ribosomal Small Subunit

A. Yu. Sosorev[1,2*]
[1]Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry RAS
[2]Moscow State University, Faculty of Physics
*e-mail: sosorev@physics.msu.ru

Despite several decades of research, the physics underlying translation – protein synthesis at the ribosome – remains poorly studied. For instance, the mechanism coordinating various events occurring in distant parts of the ribosome is unknown. Very recently, we have suggested that this allosteric mechanism could be based on the transport of electric charges (electron holes) along RNA molecules and localization of these charges in the functionally important areas; this assumption was justified using tRNA as an example.[1]

In this study, we turn to the ribosome and show computationally that holes can also efficiently migrate within the whole ribosomal small subunit (SSU). The potential sites of charge localization in SSU are revealed, and it is shown that most of them are located in the functionally important areas of the ribosome – intersubunit bridges, Fe_4S_4 cluster and the pivot linking the SSU head to the body. As a result, we suppose that hole localization within the SSU can affect intersubunit rotation (ratcheting) and SSU head swiveling, in agreement with the scenario of electronic coordination of ribosome operation. We anticipate that our findings will improve the understanding of the translation process and advance the molecular biology and medicine.

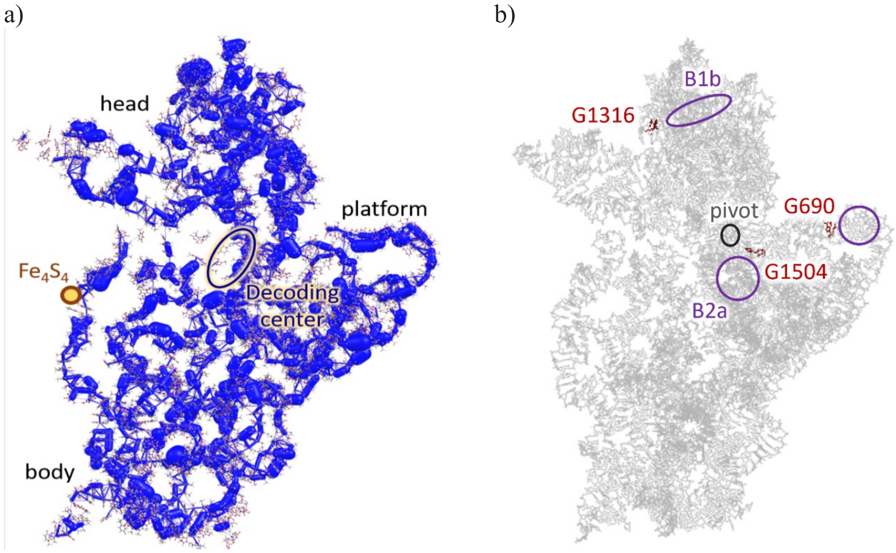


Fig. 1. (a) Transfer integrals between the nucleotides in SSU. Thicknesses of the cylinders represent the magnitudes of transfer integrals. (b) Hole localization sites within SSU (shown in red). Intersubunit bridges and pivot linking the SSU head to the body are labeled in violet and dark grey, respectively.

This work was supported by RFBR (project № 19-32-60081).

---

[1] Sosorev, A.; Kharlanov, O. *Phys. Chem. Chem. Phys.*, 2021, **23**, 7037-7047.

P-35

Inkjet printing of Organic Electrochemical Transistors with PEDOT:PSS-based Ink

Ya.O. Titova[1]*, *A.A. Trul*[1], *E.Yu. Poimanova*[1], *E.V. Agina*[1], *S.A. Ponomarenko*[1]

[1] Enikolopov Institute of Synthetic Polymeric Materials RAS
*e-mail: yaroslava.titova@ispm.ru

Inkjet printing technology is a widely used approach for producing flexible organic electronic devices and has such advantages as high speed of spot and contactless printing of functional layers of arbitrary shape and size.[1] Organic Electrochemical Transistor (OECT) is one of rather simple devices for chemo- and biosensing, which allows achieving ultrahigh sensitivity.[2] PEDOT:PSS, being an aqueous suspension of a complex of poly(3,4-ethylenedioxythiophene) with polystyrene sulfonic acid, is often used as a functional layer in OECT.[3] However, such devices often required rather high gate voltage leading to their limited stability. One of the factors influencing their electrical characteristics is uniformity and good adhesion of the printed functional layer. To improve it, surface of the substrate before printing can be modified by UV/ozone curing, plasma treatment or chemically.

In this work, influence of the modification layer on the print quality of an ink from PEDOT:PSS and conductivity of the printed spots was investigated. Si/SiO_2 wafer was used as a substrate, modification of which was carried out by (3-aminopropyl)triethoxysilane (APTS) in the gas phase after pre-treatment by oxygen plasma. The ink was made from PEDOT:PSS PH1000 adjusted by viscosity and surface tension. Uniformity of the modification layer was estimated by contact angle measurements. As a result, conditions of stable highly conducting active layer printing were found, and working OECTs were produced (Figure 1).

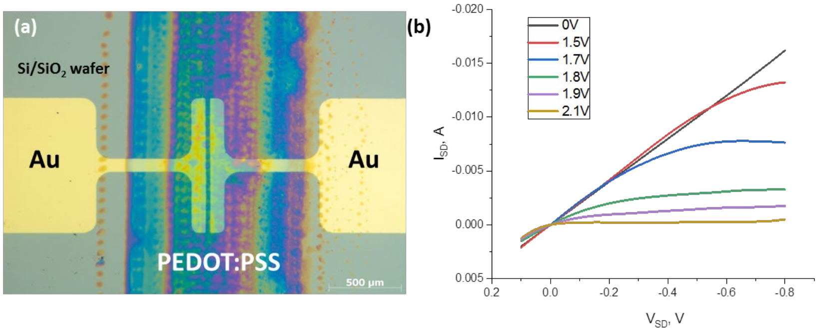


Figure 1. Optical image of fabricated OECT (a), output characteristics of the device (b).

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

---

[1] Al-Halhouli, A., Qitouqa, H., Alashqar, A., Abu-Khalaf, J. *Sensor Review*, 2018, **38**(4), 438–452.

[2] P.A. Shaposhnik, S.A. Zapunidi, M.V. Shestakov, E.V. Agina, S.A. Ponomarenko, *Rus. Chem. Rev.*, 2020, **89**(12), 1483-1506.

[3] W. Lövenich, *Polymer Science Series C* 2014, **56**, 135–143.

P-36

Synthesis of Chromophores Based on the Hydrazinylidene Cyclic Acceptor Moieties via the Reaction of Organolithium Reagents with Diazo Compounds

K.P. Trainov[1*], *R.F. Salikov*[1], *D.N. Platonov*[1], *Y.V. Tomilov*[1]

[1]N.D. Zelinsky Institute of Organic Chemistry RAS
*e-mail: trainov.tkp@gmail.com

Earlier we demonstrated that donor-π-acceptor chromophores with hydrazinylidene cyclic acceptor moieties prospective donor materials within bulk heterojunction solar cells. However, the synthesis of such chromophores was restricted by only two approaches developed. The main disadvantage of those two methods was the inability to introduce a thiophene fragment into a molecule, whereas thiophenes along with their fused polycyclic derivatives are of interest as donor parts or π-linkers. Herein we present a novel approach to the synthesis of chromophores based on various cyclic hydrazinylidene acceptor moieties via the reaction of organolithium reagents with diazo compounds. This reaction is quite exceptional due to rare electrophilic reactivity of a diazo group.

The reaction of diazocyclopentadiene **1** with various organolithium reagents gave a series of chromophores **2a-i** (Figure 1). The reaction proceeded with good selectivity and moderate to high yields despite the presence of competitive reactive groups in diazo substrates.

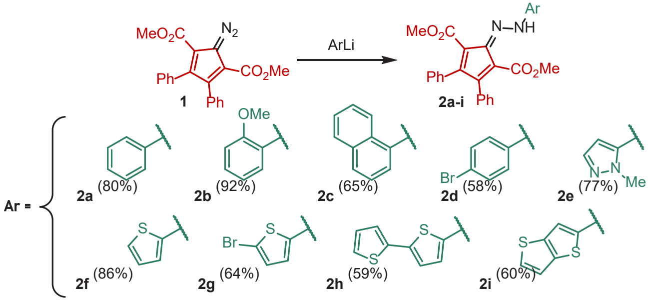


Figure 1. Reaction of diazocyclopentadiene 1 with organolithium reagents.

Furthermore, we showed that this approach affords other hydrazinylidene dyes from cyclic diazo compounds such as diazobarbituric acid, diazoindanedione and diazocyclohexadienone whose reaction with thienyllithuim gave hydrazones **3a-c** (Fig. 2).

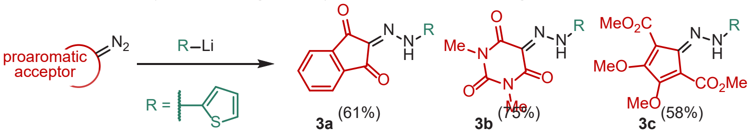


Figure 2. Reaction of thienyllithium with diazo compounds.

Using this reaction, we obtained chromophore **IDTT-HC2P** (Figure 3), which is an analogue of **ITIC**, but this compound showed poor photovoltaic properties. We associate this with bulky phenyl substituents

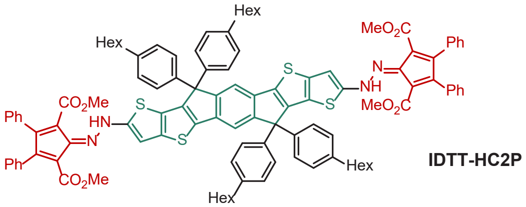


Figure 3. Structure of compound **IDTT-HC2P**

P-37

Electroluminescence Polarization Anisotropy in Organic Semiconductor Crystals

V.A. Trukhanov[1,2*], *O.V. Borshchev*[2], *S.A. Ponomarenko*[2], *D.Yu. Paraschuk*[1,2]
[1] Faculty of Physics, Lomonosov Moscow State University
[2] Enikolopov Institute of Synthetic Polymeric Materials, Russian Academy of Science
*e-mail: trukhanov@physics.msu.ru

Single crystals of thiophene-phenylene co-oligomers (TPCO) have demonstrated high potential for organic light-emitting transistors (OLETs) due to a unique combination of decent charge-carrier mobility and excellent photoluminescence (PL) efficiency[1]. The attractive feature of organic single crystals is the perfect alignment of the molecules and their transition dipole moments, which might cause electroluminescence (EL) and PL to be strongly polarized. Usually, for OLETs, organic semiconductor crystals with vertical or nearly vertical orientations of molecular transition dipole moments are used, which results in a strong waveguiding effect so that light outcoupling normally to OLET's plane is ineffective. The effects of EL anisotropy in organic semiconductor single crystals almost have not been studied, and for such studies the in-plane orientation of transition dipole moments is highly desired.

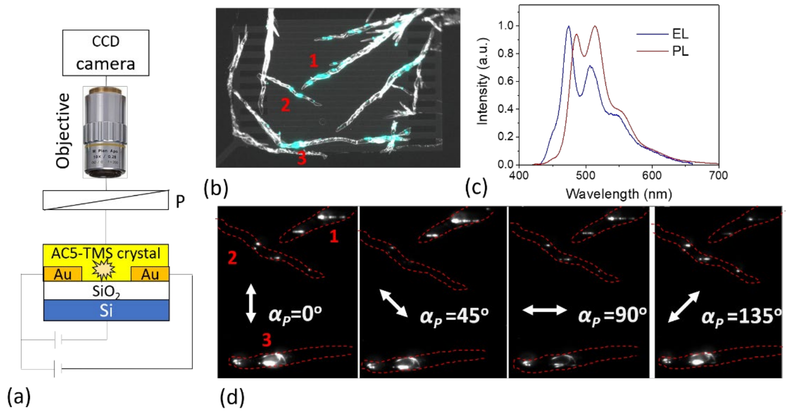


Fig. 1. Experimental setup scheme (a), OLET image under backlight with superimposed colored EL image (b), EL spectra (c), black-and-white EL images of differently oriented AC5-TMS crystals (denoted by red dashed lines) at different polarizer orientations (d).

In this work, we study EL polarization anisotropy in single crystals of 1,4-bis{5-[4-(trimethylsilyl)phenyl]thiophen-2-yl}benzene (AC5-TMS), whose PL has essential in-plane orientation[2]. For this purpose, OLETs with interpenetrating source and drain electrodes were fabricated. As Fig.1d shows, the EL intensity is minimal when the polarizer is collinear with the longest crystal edge, corresponding to the crystal **a**-axis. From X-ray diffraction data it is known that molecules are oriented almost perpendicular to **a**-axis.[2] Therefore, we conclude that EL is strongly polarized along the molecular backbone; this is in accordance with data on PL polarization anisotropy.[2]

This work was supported by RFBR (project № 18-12-00499-П).

---

[1] S. Hotta, T. Yamao, *J. Mater. Chem.*, 2011, **21**(5), 1295-1304.
[2] Mannanov A.A. (2019). *Photoluminescence and Raman Spectroscopy of Highly Ordered Organic Semiconductor Structures*. PhD Thesis, University of Groningen, Groningen, Netherlands.

P-38

Ethanethiol Detection with Operationally Stable Ultrathin BTBT-Dimers-Based OFETs

A.A. Trul[1*], *V.P. Chekusova*[1], *D.S. Anisimov*[1], *O.V. Borshchev*[1], *M.S. Polinskaya*[1],
E.V. Agina[1], *S.A. Ponomarenko*[1]

[1]Enikolopov Institute of Synthetic Polymeric Materials RAS
*e-mail: trul@ispm.ru

Modern sensor applications (air quality control, food spoilage detection or exhaled breath analysis) demand novel highly-sensitive devices having a low limit of detection (LOD) while being inexpensive, portable and having low energy consumption. Automatic alarm systems for alkanethiols detection in the concentrations above the threshold limit value are especially important due to their widespread usage as odor markers of domestic gas leakage since a lot of people suffer from a loss of smell after a coronavirus disease.

Recently we have reported OFETs based on Langmuir-Schaefer monolayers of siloxane dimer of benzothieno[3,2-b][1]benzothiophene (BTBT) that demonstrated good electrical performance and high sensitivity to toxic gases in concentrations down to dozens of ppb.[1-3] The electrodes grounding is needed for the recovery of such sensors that leads to incapability of any gases detection during this rather long process. Now, we focused on improving the OFETs operational stability without losing their sensitivity. For that purpose the influence of the aliphatic spacer length between the BTBT core and the disiloxane fragment as well as the influence of dielectric interface layers prepared from poly(methyl methacrylate) (PMMA) or octyldimethylcholosilane (ODMS) on the morphology and electrical performance of Langmuir-Blodgett (LB), Langmuir-Schaefer (LS) and spin-coating (SC) ultrathin films were studied. The best characteristics with charge-carrier mobility of 0.47 $cm^2V^{-1}s^{-1}$ were obtained for the monolayer device based on dimer with undecylic spacer fabricated by LS technique on top of the PMMA interface layer. Great operational stability leads to the good sensory ability of ethanethiol detection with LOD of 30 ppb in humid air with relative humidity up to 95% (Figure 1), what is the best one among the other portable technologies reported up to now.

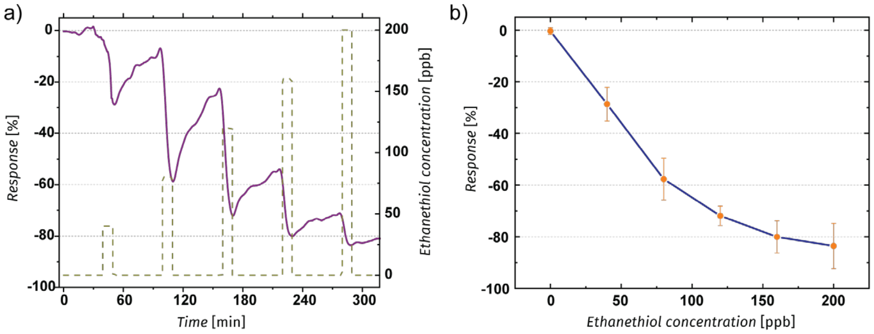


Figure 1. Full timeline of OFET response (a) and corresponding response curve (b) of ethanethiol detection in the humid air registered for the best device.

This work was supported by Russian Science Foundation (grant 19-73-30028) and was performed under financial support from Ministry of Science and Higher Education of the Russian Federation (Contract 0071-2021-0003).

---

[1] A. A. Trul, A. S. Sizov et al., *J Mater Chem C*, 2018, **6**, 9649-9659.
[2] A. S. Sizov, A. A. Trul, et al., *ACS Appl Mater Interfaces*, 2018, **10**, 43831–43841.
[3] A. A. Trul, V. P. Chekusova et al., *Sensors and Actuators B: Chemical*, 2020, **321**, 128609.

Long Exciton Diffusion Lengths in Non-Fullerene Acceptor Solar Cells: a Kinetic Monte Carlo Study

W. Yang[1*], *S. Karuthedath*[1], *J.F. Gorenflot*[1], *F. Laquai*[1]

[1]Kaust Solar Center, King Abudullah University of Science and Technology
*e-mail: wenchao.yang@kaust.edu.sa

Non-fullerene acceptors (NFA) have been widely used in the preparation of high efficiency organic solar cells due to their strong complementary absorption and low energy losses properties. The long exciton diffusion lengths in NFAs also greatly contribute to the efficient exciton dissociation and charge generation. To find the domainat factors for exciton diffusion, in this work we used kinetic Monte Carlo (KMC) method to simulate the exciton dynamics in a series of NFA materials obtained by the time resoloved photophysical measurements. With experimentally extracted parameters such as the exciton lifetime and the exciton-exciton annihilation rate, the measured exciton decay dynamics are well reproduced by KMC simulation (Fig.1), from which the exciton hopping rate and energetic disorder are determined. It is found that disorders are small and in the range of in the range of 30-40 meV, and the exciton hopping rate varies approximately as the square of the diffusion constant, which are consistent with the further calculated long exciton diffusion length.

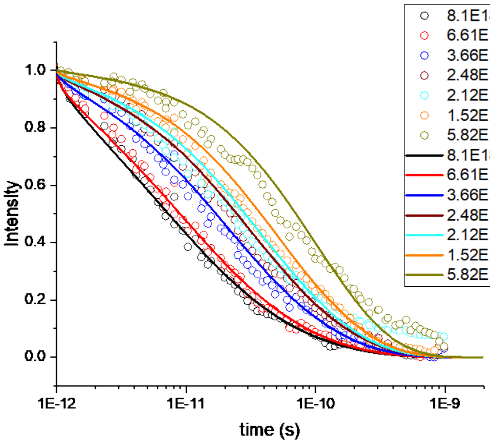


Fig. 1. The Exciton decay dynamics of the NFA material ITIC as measured by TRPL experiments (circles) and the corresponding KMC simulations (solid curves) for different initial excitation density (in units of cm^{-3}). The further calculated exciton diffusion length is 19 nm, which is comparable to the experimental extracted one of 17 nm.

P-40

Synthesis and Properties of the New Linear Polymers Based on Annelated Structures

E.A. Zaborin[1*], *O.V. Borshchev*[1], *M.S. Skorotetcky*[1], *S.A. Ponomarenko*[1,2]

[1]Institute of Synthetic Polymer Materials RAS
[2]Moscow State University, Department of Chemistry
*e-mail: zaborin@ispm.ru

Fast progress in the development of new organic semiconducting materials for organic field effect transistors (OFETs) is associated with various annelated compounds among which fused phenylene-thiophene (benzothieno[3,2-b]benzothiophene (**BTBT**) derivatives) and thienothiophene-based (tetrathienoacene (**TTA**) derivatives) molecules have been widely investigated and shown to be promising.[1]

Recently, new organic semiconductors, based on various octyl-substituted TTA derivatives were obtained.[1,2] Organosilicon dimer based on BTBT[3] was obtained to form a monolayer thin film with excellent electrical performance.

Polymers based on annelated structures are poorly studied though seem to be very promising in printing/flexible electronics for OLED, OFET and solar cell perfomances.

In this work we obtained a range of new linear polymers based on **BTBT** and **TTA** derivatives with an increased ability to self-assemble due to intra- and intermolecular interactions, as well as high flexibility due to alkyl spacers.

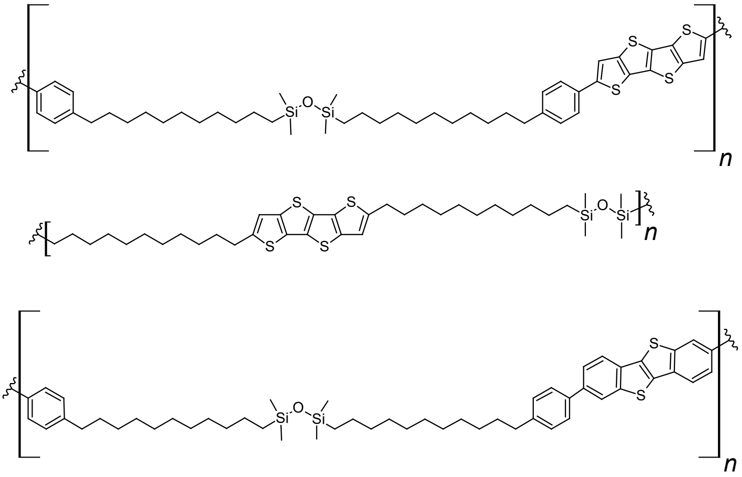


Fig.1 Polymers, based on **TTA** and **BTBT**

This work was performed under financial support from Ministry of Science and Higher Education of the Russian Federation (Contract № 0086-2019-0006).

---

[1] M.S. Skorotetcky, et al. Simple synthesis of alkyl derivatives of tetrathienoacene and their application in organic field-effect transistors.. Journal of Materials Chemistry C, 2021

[2] O.V. Borshchev, et al. Synthesis, Characterization and Organic Field-Effect Transistors Applications of Novel Tetrathienoacene Derivatives. Dyes and Pigments, 2020

[3] A.A. Trul, et al. Organosilicon dimer of BTBT as a perspective semiconductor material for toxic gas detection with monolayer organic field-effect transistors. Journal of Materials Chemistry C. 2018

P-41

Application of Solvents and Solvent Mixtures to Control the Bulk-Heterojunction Morphology

S.S. Ghosh[1*]

[1]Department of Physics, KBCNM University
*e-mail: ssghosh@nmu.ac.in

In this presentation, I would explain the application of different solvents and various solvent mixtures for application in bulk-heterojunction moroph† control for application in solar cell and organic slight emitting diodes. Studies on polymer and small molecules mixed with fullerene derivatives and non-fullerene (organic and inorganic) materials will be presented. The results on rapid spin coating method and ultraonic spray coating method having large area coating potential will be discussed. Simulation results supported by experimental data will presented on the above materials, methods and applications. Mixed solvent evaporation dynamics simulation during film drying will be presented to explain the experimental results. I would basically present my work in the last 10-12 years on solvents, solvent mixtures, for various organic materials, mixtures and methods for application in organic optoelectronics.

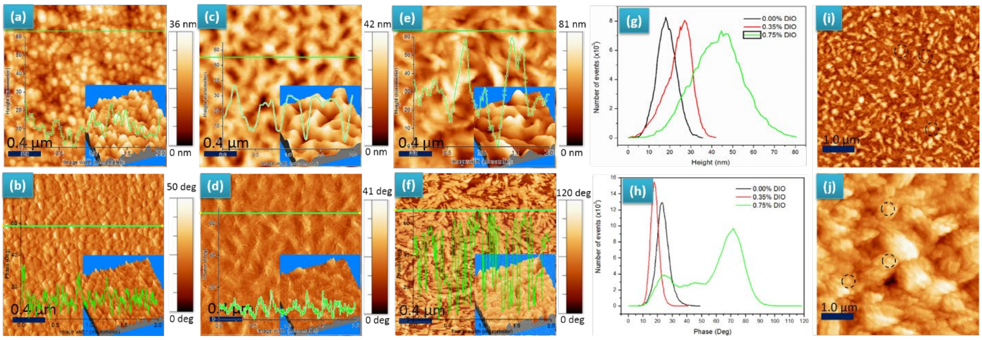


Figure 1. Atomic Force Microscopy images of the bulk-heterojunction films with different solvent mixtures and the histograms are shown.

This work was partially supported by DAE-BRNS through the project number: 34/14/12/2017-BRNS/34287. I am thankful to Prof. Jaydeep V. Sali, India; Prof. Ifor Samuel, UK and collaborators.

P-42

Optoelectronic Properties Of Spiro[4.4]nonatetraen Based Hydrocarbons

K. M. Shepovalov[1], *R.Y. Peshkov*[1], *E. Benassi*[1], *E. A. Mostovich*[1]*

[1]Novosibirsk State University, laboratory of organic electronics
*e-mail: chemmea@gmail.com

Spiroaromatic molecular systems attract significant attention as building blocks for organic electronics materials.[1,2] Having several unique properties because of their intrinsic 2D-, or 3D-molecular structure and high rigidity these materials are found to be promising. Current investigations on spiroaromatic compounds were mainly devoted to the influence of substitution on their optoelectronic properties.[3] Less attention was paid to the molecular topology of the central spiroaromatic fragments.

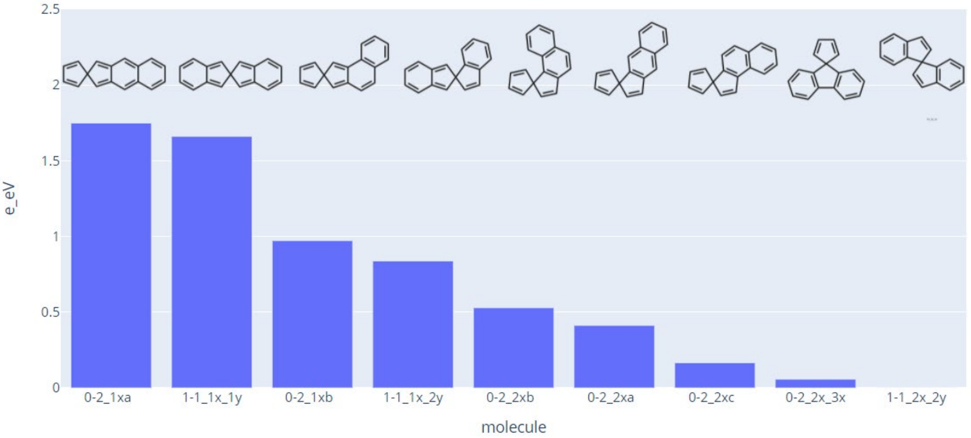


Figure 1 - Relative difference in total electron energy of molecular models

Here, we computationally investigated the charge and energy transfer properties (electronic, vibrational structures of the ground, the first singlet/triplet states, and reorganization energy) of pure hydrocarbon spiroaromatic models based on spiro[4.4]nonatetraen and differ by the number (n=0, 1, 2) and position of condensed benzene rings.

This work was supported by Russian Science Foundation (project № 19-13-00327) and Ministry of Science and Higher Education of Russian Federation project No FSUS-2020-0036.

---

[1] Ostroverkhova O. *Organic Optoelectronic Materials: Mechanisms and Applications Chem. Rev.* 2016, **116**(22), 13279–13412.

[2] Forrest S. R., Thompson M. E. *Introduction: Organic Electronics and Optoelectronics Chem. Rev.* 2007, **107**(4), 923–925.

[3] Saragi T. at al *Chem. Rev.* 2007, **107**(4), 1011–1065

Author index

A

Abashev, G.G. 34 58
Abramov, A.A. 40 53
Aeppli, G. 19
Agina, E.V. 40 53 64 70 76 77 82 87 90
Aleksandrov, A.E. 41 50 79
Andrienko, D. 13
Anisimov, D.S. 40 53 70 71 82 90
Averin, A.A. 50

B

Bakulin, A. 51
Balakirev, D.O. 42 54 60 63 84
Baranchikov, A.E. 41
Baranov, D.S. 66
Bässler, H. 39 81
Becker, C.S. 28 67
Benassi, E. 38 94
Berggren, M. 15
Bezsudnov, I.V. 76
Blom, P. 13
Bodnarchuk, M. 51
Borshchev, O.V. 34 43 46 49 55 61 62 71 89 90 92
Bujaldón, R. 56
Burdakov, Ya.V. 39 57 81

C

Carwithen, B. 51
Charushin, V.N. 69
Chekusova, V.P. 40 70 71 77 90
Chikineva, T.Yu. 73
Chistyakov, A.A. 79
Chukhlantseva, A.N. 58
Chuyko, I.A. 59

D

Daoulas, K.Ch. 31
Degtyarenko, K.M. 66
Demetriou, H. 19
Dmitriev, M.V. 58
Dorokhov, A.I. 80
Dyadishchev, I.V. 42 60

E

Ezhov, A.A. 41

F

Fedichkina, A.D. 73
Fedorenko, R.S. 43 61 62
Fedorov, Y.V. 32
Fedorova, O.A. 32
Feldman, E.V. 34
Felton, S. 19
Fishchuk, I.I. 39 81
Fisher, A.J. 19
Fleet, L.R. 19
Freidzon, A.Ya. 24

G

Gadirov, R.M. 66
Gavrilov, A.A. 48
Genoe, J. 39 81
Ghosh, S.S. 93
Giannakou, P. 84
Gorbunova, Yu.G. 41
Gorenflot, J.F. 91
Gusarova, E.A. 50
Guseva, D.V. 48

H

Harrison, N.M. 19
Heutz, S. 19
Hopper, T. 51

I

Inasaridze, L.N. 68
Ivanov, K.S. 35
Ivanov, V.A. 48
Ivanov, K.S. 78

K

Kadashchuk, A. 39 81
Kalinichenko, N.K. 42 54 63 84
Kalinina, M.A. 41 50 64 76
Karuthedath, S. 91
Kazantsev, M.S. 28 29 35 67 83 85
Khan, M.D. 37
Kharlanov, O.G. 34
Khmelnitskaya, A.G. 64 76
Kleymyuk, E.A. 65
Kobeleva, E.S. 66

Köhler, A. 39 81
Komarov, P.V. 48
Komolov, A.S. 46
Konstantinov, V.G. 80
Kopotilova, A.E. 69
Koptyaev, A.I. 72
Kornikov, A.I. 33
Koshelev, D.S. 73
Koskin, I.P. 28 29 67
Kotadiya, N. 13
Kovalenko, M. 51
Kozlov, M.I. 30 33 74
Kremer, K. 31
Krieg, F. 51
Krylov, V.B. 70
Kuevda, A.V. 43 61 62
Kuimov, A.D. 28 29 67 85
Kuklin, K.N. 62
Kulik, L.V. 66
Kuzmina, N.V. 50
Kuznetsov, K.M. 74

L

Laquai, F. 91
Lazneva, E.F. 46
Liakisheva, I.V. 35
Lipunova, G.N. 69
Luponosov, Yu.N. 42 47 54 59 60 63 65 84
Lypenko, D.A. 32

M

Maltsev, E.I. 32
Mannanov, A.L. 47 54
Martynov, A.G. 41
Martynov, I.V. 68
Maslennikov, D.R. 34
Metel, Yu.V. 39 81
Michels, J. 31
Min, J. 25
Mordan, A. 13
Moshkina, T.N. 69
Mostovich, E.A. 35 38 78 94
Muzafarov, A.M. 64

N

Neher, D. 21
Nevelskaya, A.I. 65
Nevostrueva, D.A. 66
Nikitenko, V.R. 37 39 57 79 81
Nosova, E.V. 69
Novikov, S.V. 36

O

Obrezkova, M.A. 42 60
Obukhov, A.E. 75

P

Paraschuk, D.Yu. 14 28 34 43 47 49 54 61 62 80 89
Peregudova, S.M. 54 59
Peshkov, R.Yu. 35 38 78 94
Platonov, D.N. 88
Poimanova, E.Yu. 70 82 87
Polinskaya, M.S. 71 90
Ponomarenko, S.A. 18 34 40 42 46 47 49 53 54 55 59 60 61 62 63 64 65 70 71 76 82 84 87 89 90 92
Popova, A.A. 66
Pshenichnikov, M.S. 47
Pshenichnyuk, S.A. 46
Puigdollers, J. 56

R

Raul, B.A.L. 47
Resel, R. 17
Riesebeck, T. 35
Robaschik, P. 19
Rudyak, V.Yu. 48

S

Sachkov, Yu.I. 72
Salikov, R.F. 44 88
Samburskiy, D.E. 78
Samorì, P. 20
Saunina, A.Yu. 79
Savchenko, P.S. 47 54
Saxena, R. 39 81
Scheblykin, I.G. 26
Shaposhnik, P.A. 70 82
Shepovalov, K.M. 35 38 94
Shklyaeva, E.V. 58

Shkunov, M. 84
Shumilov, N.A. 28 83
Shundrina, I.K. 28 85
Skolyapova, A.D. 35
Skorotetcky, M.S. 49 55 70 71 92
Sobolev, V.S. 46
Solodukhin, A.N. 42 47 59 60 84
Sonina, A.A. 28 29 67 85
Sosorev, A.Yu. 34 49 62 86
Soukeras, D. 19
Sukhikh, A.S. 66
Sukhorukova, P.K. 54 63
Surin, N.M. 42 47 55 60
Svidchenko, E.A. 42 54 60

T

Tameev, A.R. 32 36 41 50 79
Tcelykh, L.O. 73
Titova, Ya.O. 87
Tokarev, S.D. 32
Tomilov, Y.V. 44 88
Torsi, L. 16
Trainov, K.P. 88
Travkin, V.V. 72
Troshin, P.A. 68
Trukhanov, V.A. 28 43 89
Trul, A.A. 40 53 65 70 71 77 82 87 90
Trusov, M.A. 45
Tseng, H.H. 19
Tung, S.-H. 48

U

Utochnikova, V.V. 23 30 33 73 74
Uvarov, M.N. 66

V

Vashchenko, A.A. 30 74
Vasyanin, A.N. 58
Velasco, D. 56
Vener, M.V. 34

W

Wetzelear, G.-J. 13
Wu, Z. 19
Wu, W. 19

Y

Yang, W. 91

Z

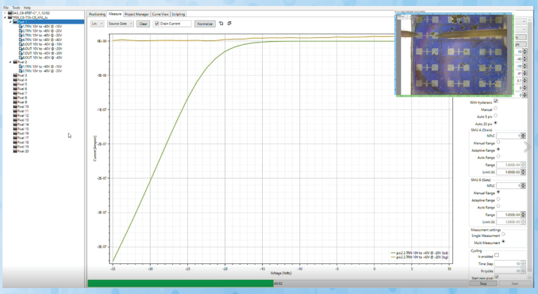
Zaborin, E.A. 92
Zavyalova, E.G. 70
Zhang, J. 31
Zvaigzne, M.A. 79
Zvyagina, A.I. 41 50

ProbeStation 100

Fully-automated low-cost probe-station designed for laboratory use and perfectly suited for semiconductors studies

Key features

- Compact design for glove-box installation
- Fully automated sample holder for fast characterization
- High accuracy current measurements with fully triaxial connectors
- Multiple-sample testing in continuous mode
- One-click measurements with user-defined scripts of the devices array
- Up to 4 semi-automated probes
- Digital microscope with LED lighting
- External LCD for probes positioning
- Keithley compatible software
- 2D sample positioning with trackball
- Software for measurement automatization
- Automatic FET parameter extraction (mobility, threshold voltage, etc.)



ProbeStation software

Additional options

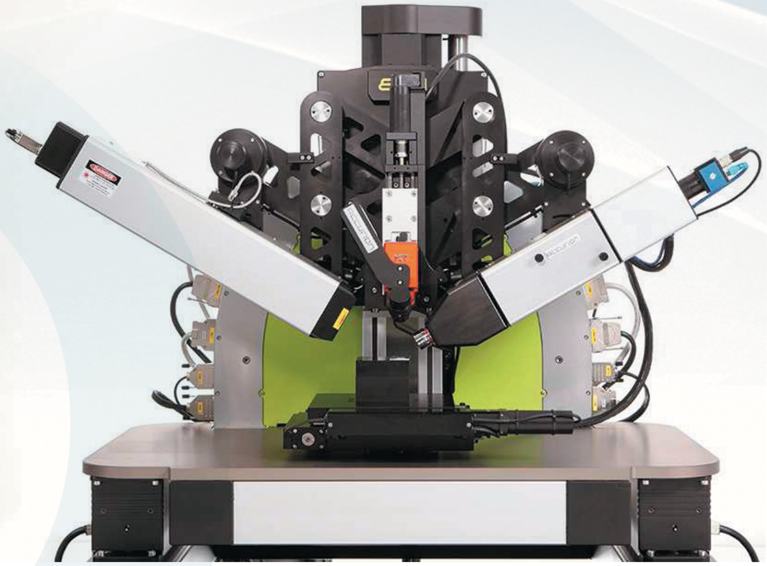
- Extra probes (4-wire sense)
- Custom sample holders
- Glove-box installation
- Keithley semiconductor analyzer
- Software extension for other semiconductor analyzers

PRINTELTECH
PRINTED ELECTRONICS TECHNOLOGIES

☎ +7 (495) 332-58-88
http://www.printeltech.com
✉ sales@printeltech.com

Profsoyuznaya st. 70,
bld.1, office 410
117393 Moscow, Russia


NIR
MIR
VIS
NIM
HSH
neaSNOM
nea spec
nano-FTIR

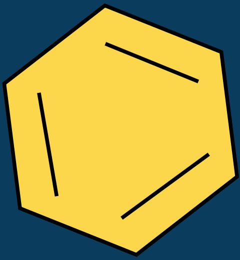


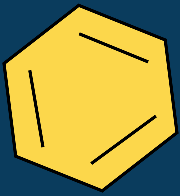
RSF

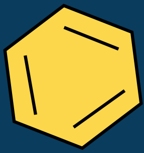
Russian
Science
Foundation

imc

INDUSTRIAL MONITORING
AND CONTROL







PRINTELTECH
PRINTED ELECTRONICS TECHNOLOGIES

Printed Electronics Technologies LLC
117393 Moscow, Russia
Profsoyuznaya st. 70, bld.1, office 410

☎ Phone: +7 (495) 332-58-47
http://www.printeltech.com
✉ sales@printeltech.com