3rd INTERNATIONAL FALL SCHOOL ON ORGANIC ELECTRONICS – 2016 (IFSOE-2016)

Organizers

Division of Chemistry and Material Science of Russian Academy of Sciences

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)

Russian Science Foundation (RSF)

Russian Foundation for Basic Research (RFBR)

Federal Agency of Scientific Organizations

Scientific program

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

2) ***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 Chairs

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School-conference program

The 3rd International Fall School on Organic Electronics – 2016 Time Schedule

	Sunday *September 18th*	**Monday** *September 19th*	**Tuesday** *September 20th*	**Wednesday** *September 21th*	**Thursday** *September 22th*	**Friday** *September 23th*	
	Conference	***School***				***Conference***	
9:00		Valentine Ananikov	Dongge Ma	Maxim Pschenichnikov	Mario Caironi	Transfer to Innovative Nanotechnology Center “Technospark“	9:00
10:00		Joji Ohshita	Dan Credgington	Henning Sirringhaus	Fabio Biscarini		10:00
11:00	Visit to Kolomenskoe Museum (optional) Lunch Registration at ISPM RAS 16:00 departure to Conference site	**Coffee-break**				Denis Kovalevich	11:00
		Mikhail Bochkarev	Andriy Zhugayevych	Koen Vandewal	Souren Grigorian	Chuck Milligan	
12:00						Viktor Zadkov	12:00
		Andrei Shevelkov	Mikhail Nechaev	Alexei Komolov	Stephan Kirchmeyer	**Coffee-break**	
13:00		Artem Bakulin	David Vanden Bout	Peter Thiesen		Alexander Mityashin	13:00
		Lunch				Boris Galkin	
14:00						Oral talks 5	14:00
		Conference				Lunch Excursion to Innovative Nanotechnology Center “Technospark“	
15:00		Oral talks 1	Oral talks 2	Oral talks 4	Trip to Zvenigorod (optional) Sport activities (horse riding)		15:00
16:00							16:00
		Coffee-break				**Closing ceremony**	
17:00	**Hotel arrival.** **Registration**	Poster session 1	Individual discussions	Poster session 2		**Departure to Moscow**	17:00
18:00							18:00
19:00	**Dinner**				**Conference dinner**		19:00
	School	Evening lecture Sport activities (swimming pool, wellness, spa)	Moscow sightseeing tour	Evening lecture Sport activities (swimming pool, wellness, spa)			
20:00	**School opening.** **Keith Stevenson**						20:00
21:00	Welcome-party						21:00
22:00-22:30							22:00-22:30

Sunday, September 18th

11:00 – 16:00	**Visit to Kolomenskoe Museum (optional)** **Registration at ISPM RAS. Departure to conference site**
19:00 – 20:00	**Dinner**
20:00 – 20:15	**School opening**
20:15 – 21:15	**T-1**. *Keith Stevenson.* Spatially-resolved measurements of organic semiconductor interfaces
21:15 – 22:30	**Welcome-party**

Monday, September 19st

8:00 – 9:00	**Breakfast**
9:00 – 10:00	**T-2**. *Valentine Ananikov.* Catalytic reactions for preparation of complex organic molecules with atomic precision
10:00 – 11:00	**T-3**. *Joji Ohshita.* Group 14 element chemistry for organic optoelectronic materials
11:00 – 11:30	**Coffee-break**
11:30 – 12:30	**T-4**. *Mikhail Bochkarev.* Features of luminescence of organic compounds of rare earth metals
12:30 – 13:00	**I-1**. *Andrei Shevelkov.* Chemistry of Perovskite Solar Cells
13:00 – 13:30	**I-2**. *Artem Bakulin.* Structural and electronic dynamics in hybrid perovskite materials for photovoltaic and light-emitting devices
13:30 – 15:00	**Lunch**
15:00 – 15:15	**O-1**. *Alexander Dudnik.* Direct C-H arylation polymerization toward sustainable synthesis of conjugated polymers for high performance organic electronics
15:15 – 15:30	**O-2**. *Evgeny Mostovich.* 9H-Fluorene-9-ylidene-caped small molecules: toward rational design of conformational dependent optical properties for organic optoelectronics
15:30 – 15:45	**O-3**. *Yuriy Luponosov.* Design of donor-acceptor oligomers for solution-processed organic solar cells
15:45 – 16:00	**O-4**. *Alexey Tereshchenko.* Nanostructured organosilicon luminophores – large scale synthesis and application in organic photonic and optoelectronic devices
16:00 – 16:15	**O-5**. *Maria Kotova.* Resistive switches in composite structures based on organic dyes and colloidal nano plates CdSe
16:15 – 16:30	**O-6**. *Alexander Shokurov.* Selective mercury sensor model based on crown-substituted hemicyanine dye monolayer at air/water interface
16:30 – 17:00	**Coffee-break**
17:00 – 18:30	**Poster session 1 (*P-1 – P-27*)**

19:00 – 20:00	**Dinner**
20:00 – 21:00	**Evening lecture.** *Maxim Pschenichnikov.* How to write a scientific paper
20:00 – 22:30	**Sport activities**

Tuesday, September 20st

8:00 – 9:00	**Breakfast**
9:00 – 10:00	**T-5**. *Dongge Ma.* Organic semiconductor heterojunctions and their application in OLEDs
10:00 – 11:00	**T-6**. *Dan Credgington.* Recombination and spin in printable OLEDs
11:00 – 11:30	**Coffee-break**
11:30 – 12:30	**T-7**. *Andriy Zhugayevych.* First-principle modeling of energy and charge transport in organic semiconductors
12:30 – 13:00	**I-3**. *Mikhail Nechaev.* QM modeling of materials for organic electronics
13:00 – 13:30	**I-4**. *David Vanden Bout.* Spectroscopy of single conjugated polymers and aggregates
13:30 – 15:00	**Lunch**
15:00 – 15:15	**O-7**. *Alexandra Freidzon.* Multireference quantum chemistry in organic electronics
15:15 – 15:30	**O-8**. *Yulia Krupskaya.* Band-like transport and magnetic ions at organic charge transfer interfaces
15:30 – 15:45	**O-9**. *Maxim Kazantsev.* Highly-emissive solution-grown furan/phenylene co-oligomer single crystals
15:45 – 16:00	**O-10**. *Olga Parashchuk.* Dopant-enhanced photoluminescence in solution processed semiconducting single crystals
16:00 – 16:15	**O-11**. *Vladimir Bruevich.* Thiophene-phenylene co-oligomer single crystals unintentionally doped by longer co-oligomers: optical and electrical properties
16:15 – 16:30	**O-12**. *Igor Fedorov.* Mono- and tri-methine carbocyanine dye J-aggregates: Influence of aggregation promoters on optical and stability properties
16:30 – 17:00	**Coffee-break**
17:00 – 18:00	**Individual discussions**
18:15 – 19:00	**Dinner**
19:00 – 23:00	**Moscow Sightseeing tour**

Wednesday, September 21st

8:00 – 9:00	**Breakfast**

9:00 – 10:00	**T-8**. *Maxim Pschenichnikov.* Excitons in organic semiconductors
10:00 – 11:00	**T-9**. *Henning Sirringhaus.* Device physics of organic transistors
11:00 – 11:30	**Coffee-break**
11:30 – 12:30	**T-10**. *Koen Vandewal.* Charge-transfer states for organic solar cells, OLEDs and NIR photo-detectors
12:30 – 13:00	**I-5**. *Alexei Komolov.* Electron spectroscopy studies of organic electronics materials
13:00 – 13:30	**O-13**. *Peter Thiesen.* Current trends in spectroscopic imaging ellipsometry and brewster angle microscopy
13:30 – 15:00	**Lunch**
15:00 – 15:15	**O-14**. *Oleg Kozlov.* Enhanced exciton harvesting in rubrene:C60 heterojunctions
15:15 – 15:30	**O-15**. *Fallon Colberts.* Water-based processing of electro-active layers in organic solar cells
15:30 – 15:45	**O-16**. *Gaël Heintges.* The effect of branching in a semiconducting polymer on the efficiency of organic photovoltaic cells
15:45 – 16:00	**O-17**. *Qiang Wang.* Structure-property relationships for bis-diketopyrrolopyrrole molecules in organic photovoltaics
16:00 – 16:15	**O-18**. *Andrey Sosorev.* Stepwise change of conjugated polymer:acceptor blend properties with acceptor electron affinity
16:15 – 16:30	**O-19**. *Artem Bakirov.* Structure of star-shaped D–π–A oligothiophenes in solid state and in thin films
16:30 – 17:00	**Coffee-break**
17:00 – 18:30	**Poster session 2 (*P-28 – P-63*)**
19:00 – 20:00	**Dinner**
20:00 – 21:00	**Evening lecture.** *Dmitry Paraschuk.* Basic concepts in organic electronics
20:00 – 22:30	**Sport activities**

Thursday, September 22th

8:00 – 9:00	**Breakfast**
9:00 – 10:00	**T-11**. *Mario Caironi.* Printed polymer and hybrid transistors: from fundamentals to high frequency devices
10:00 – 11:00	**T-12**. *Fabio Biscarini.* Electrolyte-gated organic field effect transistors: fundamentals and applications to biosensing
11:00 – 11:30	**Coffee-break**
11:30 – 12:30	**T-13**. *Souren Grigorian.* Real time X-ray studies of organic thin films

12:30 – 13:30	**T-14**. *Stephan Kirchmeyer.* Organic and printed electronics: materials, technologies, opportunities and challenges
13:30 – 15:00	**Lunch**
15:00 – 19:00	**Trip to Zvenigorod (optional)** **Sport activities**
19:00 – 22:30	**Conference dinner**

Friday, September 23th

8:00 – 9:00	**Breakfast**
9:00 – 11:00	**Transfer to Innovative Nanotechnology Center “Technospark“**
11:00 – 11:30	**I-6**. *Denis Kovalevich.* Russia’s position in the emerging global industry of flexible electronics
11:30 – 12:00	**I-7**. *Chuck Milligan.* Organic thin film transistors industrialisation and applications
12:00 – 12:30	**I-8**. *Victor Zadkov.* Harnessing plasmonic nanoparticles for solar cells
12:30 – 13:00	**Coffee-break**
13:00 – 13:30	**I-9**. *Alexander Mityashin.* Towards high performance organic semiconductor films on arbitrary substrates
13:30 – 14:00	**I-10**. *Boris Galkin.* Russian flexible electronics centre – a platform for prototyping and small scale manufacturing
14:00 – 14:15	**O-20**. *Dmitry Yakovlev.* Towards high performance organic – inorganic perovskite photovoltaics with CNT based top electrode
14:15 – 14:30	**O-21**. *Vicktoria Zheltova.* Drivers of the development of organic electronics as a framework for the applied laboratory
14:30 – 16:30	**Lunch** **Excursion to Innovative Nanotechnology Center “Technospark“**
16:30 – 17:00	**Closing ceremony**
17:00 – 17:15	**Departure to Moscow**

Poster session 1

Monday, September 19th, 17:00

Anisimov, Daniil S.	P1	Ambipolar transport in single crystal field-effect transistors based on thiophene-phenylene co-oligomers
Bakiev, Artur N.	P2	New chromophores based on combination of thiophene, ethylenedioxythiophene and carbazole fragments: synthesis and optoelectronic properties
Begantsova, Yulia E.	P3	Electroluminescent polynorbonenes with pendant ionic iridium(III) complexes as perspective emitters for OLEDs
Bhattacharyya, Sohini	P4	A Single crystalline organic semiconductor with mechanochromic and solvatochrmic properties and facile metal coordination
Borshchev, Oleg V.	P5	Nanostructured organosilicon luminophores for organic optoelectronics
Brackmann, Stefan	P6	In pursuit of high efficiency hybrid devices: Functionalization of Gallium nitride surfaces
Dominskiy, Dmitry I.	P7	Thiophene-phenylene co-oligomer single crystals: effect of end groups
Emelianov, Aleksei V.	P8	TCTA based single-molecular organic field effect transistors with single-walled carbon nanotubes contacts
Feldman, Elizaveta V.	P9	Correlating the low-and high-frequency vibrations of thiophene-phenelyene co-oliogemer single crystal with its lattice parameters
Frantseva, Ekaterina S.	P10	Synthesis and physico-chemical properties of 1,4-bis(5-arylfuran-2-yl) benzenes
Glushkova, Anastasia V.	P11	Large-area ultrathin single crystal films as an active layer for organic FETs
Grodd, Linda Sabrina	P12	In situ grazing incidence X-ray diffraction of polymer-fullerene thin films under thermal treatment
Guseynov, Abdul-Akim D.	P13	Analysis of $ASnI_3$ ($A=CH_3NH_3$+ or Cs+) and doped Cs_2SnI_6 perovskite-like structures
Gushchin, Maxim G.	P14	Deposition of electroactive molecules in micro and nano gaps
Heuvel, Ruurd	P15	Energy level tuning of PPDTBT polymers: towards high V_{oc}, low energy loss solar cells
Hietzschold, Sebastian	P16	Solution cast nickel oxide thin films as efficient hole extraction layers in organic electronics
Ilichev, Vasiliy A.	P17	Low LMCT state lanthanide complexes as luminophores in phosphorescent and NIR-emitting OLEDs
Ilicheva, Alena I.	P18	Novel binuclear copper(I) complexes as perspective emitters for OLEDs
Kleymyuk, Elena A.	P19	Synthesis and properties of dendritic organosilicon luminophores with various central acceptor groups
Kolesnikov, Efim A.	P20	Obtaining of the thin layers of $CH_3NH_3PbI_3$ and ZnO for application in solar power engineering
Komissarova, Ekaterina A.	P21	Synthesis of novel pyrimidine derivatives of D-[π]-D type containing heterocycles and TTF moieties

Konstantinov, Vladislav G.	P22	Solid photoluminescence standard based on an organosilicon luminophore
Koskin, Igor P.	P23	Theoretical study of annulation effect in O- and S-containing five-ring heterocyclic rod-like molecules on their optical and electronic properties
Krivtsova, Evgenia D.	P24	Novel conjugated organosilicon oligomers based on 2,1,3-benzothiadiazole
Kunz, Alexander	P25	Reduced charge carrier trapping by controlled polymer blend phase dynamics
Malakhova, Yulia N.	P26	Polyaniline/polyethylene oxide memristors with planar thin-film or 3D fibrous architecture
Mannanov, Artur A.	P27	Photoluminescence anisotropy in organic semiconducting single crystals

Poster session 2 Wednesday, September 21th, 17:00

Mannanov, Artur L.	P28	Highly soluble and thermally stable star-shaped oligomer for organic solar cells
Maslennikov, Dmitry R.	P29	Surface-enhanced Raman spectroscopy of semiconducting monolayers
Müller, Lars	P30	Charge-transfer – solvent interaction predefines doping efficiency in p-doped P3HT-films
Naumov, Artem I.	P31	Efficient modeling of conjugated polymers for electronics and energy storage
Platonova, Elena O.	P32	Red light-emitting polynorbornenes with cyclometaled iridium(III) complexes in side chains
Poimanova, Olena Yu.	P33	Solution-grown large-area ultrathin films of α,α’-dihexylquinquethiophene for organic field-effect transistors
Polinskaya, Marina S.	P34	Synthesis and properties of novel organosilicon derivative of [1]benzothieno[3,2-b][1]-benzothiophene
Pushkarev, Anatoly P.	P35	Sensitization of NIR emission of Nd^{3+} by Zn-containing Schiff base complex
Romashkin, Alexey V.	P36	Development of nanoscale contacts for organization and study low-molecular channel OFET
Rörich, Irina	P37	Role of energetic disorder and traps on exciton lifetime in conjugated polymers
Saunina, Anna Yu.	P38	Effect of microscopic Coulomb interactions on the mobility of charge carriers in disordered organics
Schneeweis, Arno Paul Wilhelm	P39	Di(benzothieno)thiazines – New Electron Rich Organic Molecules
Schönbein, Ann-Kathrin	P40	Kinetic Modeling of PPV Polymerization via Gilch
Selivanova, Daria G.	P41	New π-conjugated systems, containing prop-2-en-1-one, 2-aminopyrimidine and 2-(1H-pyrrol-1-yl)pyrimidine moieties
Sizov, Alexey S.	P42	Electrical characterization of self-assembled monolayer field-effect transistors based on Langmuir films of organosilicon conjugated oligomers

Skorotetcky, Maxim S.	P43	New nanostructured organosilicon luminophores for organic photonics
Solodukhin, Aleksandr N.	P44	Novel donor-acceptor oligomers of different architecture based on triphenylamine and carbazole for organic photovoltaics
Temiz, Cansel	P45	Relation between supramolecular structure and the charge and excited state dynamics in organic materials
Toropynina, Viktoriya Yu.	P46	Unsymmetrical push-pull oligomers based on triphenylamine: synthesis and properties
Trukhanov, Vasiliy A.	P47	Modeling of the photocurrent in organic field-effect transistors
Trul, Askold A.	P48	Highly stable ultrathin OFETs from siloxane dimers of BTBT
Willems, Robin Egidius Marinus	P49	Singlet fission in pentacene solar cells
Zhukov, Yurii M.	P50	Oxygen contents and the surface workfunction of the liquid phase deposited graphene oxide films studied by photoelectron spectroscopy
Baramygin, Aleksandr V.	P51	Conduction band electronic structure of the ultrathin films of substituted perylene and fullerene on germanium oxide surface
Panina, Yulia A.	P52	Energy level alignment in the ultra-thin layers of polar substituted phthalocyanine and phenylene-vinylene oligomer on solid substrate
Zashikhin, Georgy D.	P53	Density of the unoccupied electronic states of the films of dioctyl-substituted and of diphenyl-substituted perylenedicarboximide
Bensalem, Rechid	P54	Structure and magnetic properties of nanocrystalline mechanically alloyed Fe-10%Zn and Fe-30%Zn
Borzdun, Natalia I.	P55	Molecular dynamics simulation of P3HT helical structure in vacuo and in amorphous polymer surrounding
Dominguez, Sergio Ulises Espinosa	P56	Computational rational design of cationic polyelectrolytes with enhanced hydrogen bonding ability for electrode buffer layers
Godovsky, Dmitri Yu.	P57	New D1-A-D2-A-D1-type small molecules based on fluorobenzotri-azole acceptor and dithienosilole core donor for solution processed organic solar cells
Kuklin, Sergei A.	P58	Design and synthesis of new ultra-low bandgap thiadiazolouinoxaline based polymers for near infrared organic photovoltaic application
Labidi, Malika	P59	First-principles study of the electronic energy bands and state density of Rock-salt $Zn_{1-x}Sr_xO$ ternary alloys
Labidi, Salima	P60	Theoretical investigations of structural, electronic and thermal properties of CdO and ZnO
Rehamnia, Rabah	P61	Zn-Ni alloys electrodeposited from alkaline medium bath containing complexing agents
Postnikov, Valeriy A.	P62	Liquid–air interface solution growth and structure of large single crystals films of p-quaterphenyl and his novel terminal substituted derivatives
Lyasnikova, Maria S.	P63	The solution processed thin crystal layers formation of organic semiconducting co-oligomers on substrate

Tutorial lectures

Spatially-resolved Measurements of Organic Semiconductor Interfaces

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Chief among the key enabling technologies for making the transition from hydrocarbon based energy to renewables are electrochemical energy systems, such as rechargeable batteries, photovoltaics, photoelectrochemical cells, and fuel cells. All of these proposed systems require the optimization of three-dimensional (3D) electrode architectures to facilitate mass transport, charge transport (i.e., electron and hole mobility), and electron-transfer kinetics in order to convert and store energy. These 3D electrode architectures are actually three-phase interfaces involving several materials components that ensure contact between an electronically conducting solid phase (the electrode), and hole (ion) and electron transporting phases (e.g. the donor-acceptor absorbing layers) with co-continuous networks that facilitate rapid charge separation and transfer. As a specific example, the recent investments to explore organic photovoltaics for photonic to electrical energy conversion have facilitated several advancements including double digit power conversion efficiencies (PCEs). These advancements have come from several competing systems: polymer (donor)/fullerene (acceptor) blends, all-small molecule systems, and tandem cells. In the case of bulk polymer(donor)/fullerene(acceptor) heterojunctions (BHJ) the steady improvement in PCE has been accomplished by synthesizing polymers with low band gap and optimization of the device morphology. However, a clear correlation between energy conversion properties and compositional and morphological parameters required for rational device optimization, is lacking; The lack of direct mechanistic understanding of BHJs is a result of the dearth of ultra-sensitive, spatially resolving tools that are capable of characterizing the “buried” morphologies on the 10-20 nm scale as well as probing the chemical composition and extent of the mixed interface. This lecture will describe our devekopment of an ultra-sensitive 3D imaging methodology to study chemical composition and morphology of buried interfaces that combines Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), Atomic Force Microscopy (AFM) and Kelvin Probe Microscopy (KPM). This methodology is schematically depicted in Fig. 1.

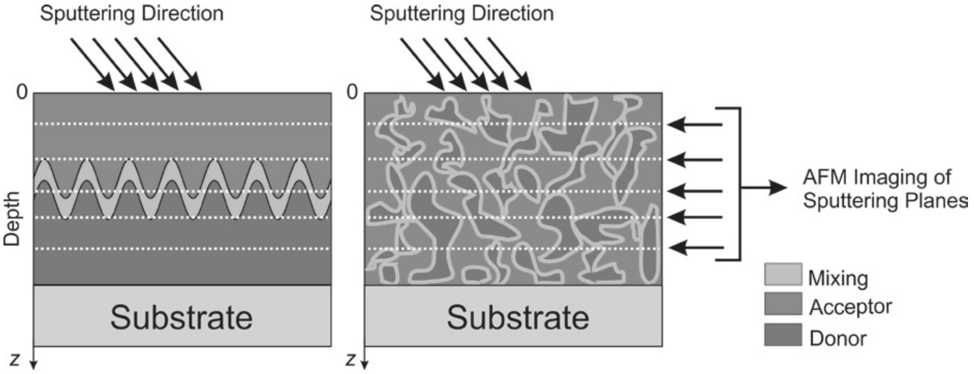

Fig. 1. Schematic illustration of TOF-SIMS depth profiling experiment on both planar (a) and bulk heterojunctions (b). The buried interfaces are revealed by sputtering and subsequently imaged using AFM (and other methods).

Catalytic reactions for preparation of complex organic molecules with atomic precision

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Fascinating development of transition metal catalysis created a new paradigm in organic synthesis towards preparation of functionalized molecules with atomic precision[1]. Detailed mechanistic studies have shown that homogeneous catalytic reactions, traditionally considered with monometallic active species, are in fact carried out in multicomponent reaction mixtures, which contain a number of metal species in solution. Participation of different metal species in the catalytic transformation initiates formation of "cocktail"-like systems[2]. Tuning of "cocktail" of catalysts provides outstanding opportunity to create dynamic and adaptive catalytic systems[3]. Heterogeneous catalysis may also involve formation of a number of active species that possess dynamic properties and interconversions on the surface[4]. A valuable direction of research is reducing the cost of metal catalysts and application of easily available metal precursors[5].

As far as catalyst dynamics and "cocktail"-like systems are concerned, an important issue is contamination of the products with traces of metal species. The topics related to construction of efficient and selective catalytic systems with traceless operation will be presented and discussed.

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[1] Ananikov V.P., Khemchyan L.L., Ivanova Yu.V., et al., *Russ. Chem. Rev.*, 2014, **83**, 885 [doi: 10.1070/RC2014v083n10ABEH004471].

[2] Kashin A.S., Ananikov V. P., *J. Org. Chem.*, 2013, **78**, 11117 [doi: 10.1021/jo402038p].

[3] (a) Ananikov V. P., Orlov N. V., Zalesskiy S. S., Beletskaya I. P., Khrustalev V. N., Morokuma K., Musaev D. G., *J. Am. Chem. Soc.*, 2012, **134**, 6637 [doi: 10.1021/ja210596w]. (b) Zalesskiy S. S., Sedykh A. E., Kashin A. S., Ananikov V. P., *J. Am. Chem. Soc.*, 2013, **135**, 3550 [doi: 10.1021/ja311258e].

[4] Pentsak E. O., Kashin A. S., Polynski M. V., Kvashnina K. O., Glatzel P., Ananikov V. P., *Chem. Sci.*, 2015, **6**, 3302 [doi: 10.1039/C5SC00802F].

[5] Ananikov V.P., *ACS Catal.*, 2015, **5**, 1964 [doi: 10.1021/acscatal.5b00072].

T-3

Group 14 element chemistry for organic optoelectronic materials

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Silicon-based compounds and polymers are of current interest, because of their interesting electronic states that are much different from the carbon analogues.[1] This lecture start with a brief introduction of the histry and fundumental properties of silicon bonding, then deals with the synthesis, properties, and optoelectronic functionalities of organosilicon compounds and polymers, mainly focusing on silole (silacyclopentadiene) derivatives. Some germole-analogues are also covered.

There has been also considerable interest in silole-containing compounds, since interesting properties of silole derivatives based on the orbital interaction between the silicon σ*- and the butadiene π*-orbital (σ*-π* conjugation) were demonstrated by Tamao, Yamaguchi, and coworkers.[2] Arising from the σ*-π* interaction, silole has the lower-lying LUMO relative to that of the carbon-analogue (cyclopentadiene), as shown in Figure 1a. The low-lying LUMO leads to sufficiently high electron-affinity of siloles, making it possible to utilize them as efficient electron-transporting layer materials for multi-layered organic light emitting diodes (OLEDs). Highly luminescent and carrier transporting properties have been also reported for silole-based compounds and polymers.

Siloles condensed with biaryls have been also extensively studied.[3] Examples include dibenzosilole and dithienosilole (DBS and DTS in Figure 1b), which are widely used as building blocks of conjugated oligomers and polymers. Usefulness of them as active materials for OLEDs, organic thin film transistors (OTFTs), and bulk hetero-junction polymer solar cells (BHJ-PSCs) is also described.

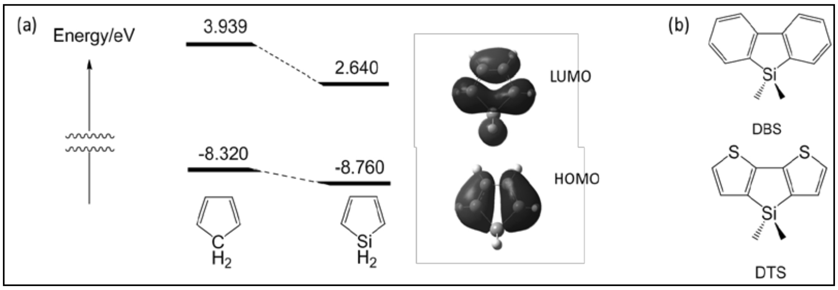

Figure 1. (a) HOMO and LUMO energy levels for cyclopentadiene and silole, derived from DFT calculations. (b) HOMO and LUMO profiles for silole, showing σ*-π* conjugation in LUMO.

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Features of luminescence of organic compounds of rare earth metals

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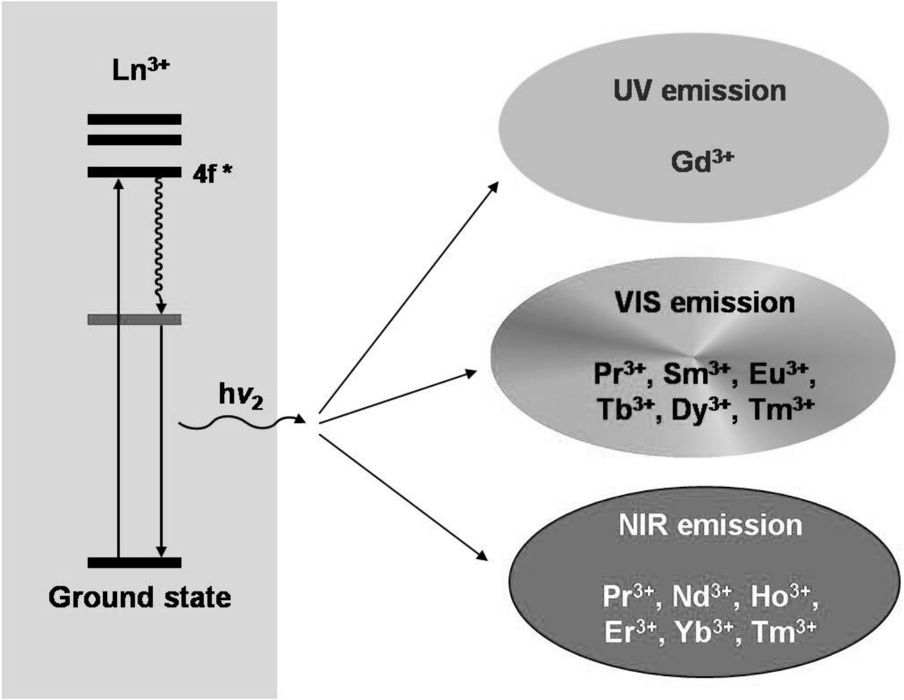
Unlike d metals, which normally do not display the metal centered luminescence, for lanthanides the metal centered emission due to f-f transition is characteristic and can be observed at room temperature for majority of inorganic and organic derivatives. The processes of photo- (PL) and electroluminescence (EL) are well studied and described in dozens of book and hundreds of reviews and original papers. In this tutorial presentation the basic points of PL and EL of organic complexes of 3 group metals including scandium and yttrium will be considered briefly. Advantages and drawbacks of lanthanide emitters as compared to organic and d metal-organic luminophores are evaluated. The main attention will be paid to the compounds emitting in UV and near IR regions. Special attention will be paid to the peculiarities of luminescence of compounds containing ytterbium, europium and samarium, which have relatively stable divalent state. Application of lanthanide complexes for realization of up-conversion is considered as well.



This work was supported by Russian Scientific Foundation (project 14-13-01158).

Organic semiconductor heterojunctions and their application in OLEDs

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Organic light-emitting diodes (OLEDs) are driven by injected charges from an anode and a cathode. Low energy barriers at electrode/organic film interfaces are desired for efficient charge injection and are generally a prerequisite to high device performance. The general methods are introducing an interfacial layer or doping organic layers at electrodes. However, as we know, the device performance is yet strongly independent on the work function of used electrode metals, which is difficult to be resolved now. More seriously, the instability caused by defects and high space electric field due to charge accumulation at the interface between electrodes and organics is detrimental to the efficiency and lifetime of OLEDs.

In addition, tandem or stacked OLED is a promising device structure that can potentially achieve both high efficiency and long operating hours. A typical tandem OLED is fabricated by vertically connecting several individual electroluminescent (EL) units together in series via the so-called charge generation layer (CGL). In tandem OLEDs, the CGL obviously plays a very important role. Therefore, how to construct an effective CGL become a key in the fabrication of high efficiency tandem OLEDs.

In this lecture, we presented the concept of the organic semiconductor heterojunctions composed of a p-type organic semiconductor and an n-type organic semiconductor, respectively, as charge injectors and CGLs in OLEDs. It is found that as charge injectors instead of metal electrode, the fabricated OLEDs show high efficiency. More attractively, the charge carrier injection is only dependent on the electric field on the heterojunction, and the metal electrodes here just play the function of providing an electric field. Therefore, the organic heterojunction injector-based OLEDs still achieve excellent EL performance even though using air- and chemistry-stable high work function metals such as Au, Ag, and Cu as contact electrodes, which is generally very difficult in conventional OLEDs. As CGLs in tandem OLEDs, we found that not only the brightness and current efficiency are doubled, but also the power efficiency is also greatly improved, which is difficult in tandem OLEDs based on general CGLs.

T-6

Recombination and Spin in Printable OLEDs

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Organic light-emitting diodes (OLEDs) are one of the biggest success stories of the organic semiconductor community. They are a direct application of carbon-based emissive molecules in commercial devices, where their unusual electronic behavior allows OLEDs to surpass the performance of many inorganic technologies. This tutorial lecture will explore the two pillars of OLED device physics – recombination and spin.

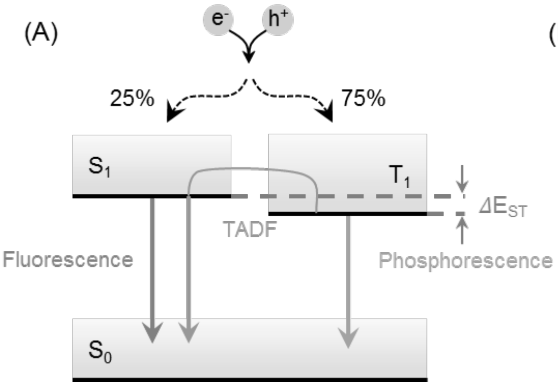

Fig. 1. Spin-dependent emission from electrically generated excitons in OLEDS. (A) Fluorescence, phosphorescence and TADF; (B) Recycling though triplet fusion. S_1 and T_1 are the lowest-energy singlet and triplet excitonic states, S_0 is the ground state.

From a discussion of electron-hole recombination, exciton formation and control of the recombination zone in OLED devices, we will cover the four primary approaches for achieving efficient emission from electrically-generated excitons: Fluorescence,[1,2] Phosphorescence,[3] Thermally-activated Delayed Fluorescence[4] (TADF) and Triplet Fusion (Fig. 1A&B).[5] All are crucially limited by how they utilize the energy stored in spin-1 (triplet) excitons and the energetic offset between singlet and triplet states, ΔE_{ST}. The number, lifetime and eventual fate of triplets has far-reaching implications not only for OLED performance, but also OLED stability, and is one reason why efficient, long-lived deep blue organic emitters remain elusive after nearly three decades of searching.

Financial support from the Royal Society is gratefully acknowledged.

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First-principle modeling of energy and charge transport in organic semiconductors

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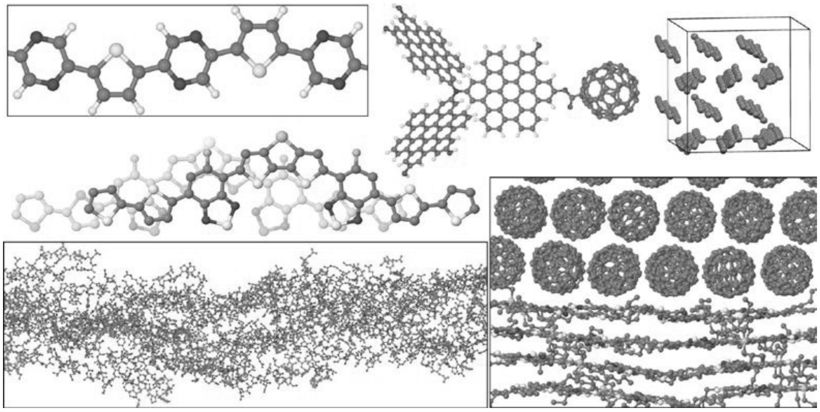

Fig. 1. Diversity of π-conjugated systems: their common feature is a strong interplay between structural and electronic degrees of freedom.

One of the key processes determining functional properties of organic semiconductors in optoelectronic devices is charge and energy transport. Being a dynamic cooperative phenomenon, this process presents a notorious challenge for theoretical description. At the other side, complex structure and multiscale inhomogeneity of real devices limit efficiency of in-depth experimental studies augmented with empirical models. That is why accurate modeling of energy and charge transfer processes has always been of high importance for research in organic electronics, particularly for establishing relationships between chemical structure of constituents and functional properties of bulk systems.[1]

In this tutorial lecture we will give an overview of first-principle modeling (i.e. based only on fundamental interactions between constituting atoms, no ad hoc assumptions or empirical knowledge) of charge carrier and Frenkel exciton transport in organic semiconductors. The primary focus is on accuracy: major sources of errors, relation to observable macroscopic properties, and some challenging systems evading an accurate description will be discussed. The emphasis is on strong interplay between structural and electronic degrees of freedom, which is a distinguishing feature of π-conjugated systems, while relevant for some inorganic/hybrid semiconductors as well.

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Excitons in Organic Semiconductors

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Organic electronic devices are based on organic semiconductors which combine attractive properties of organic materials with semiconducting behavior. The elementary excitation in these materials is a so-called “Frenkel exciton” – a strongly bound pair of negative (electron) and positive (hole) charges. As a result, organic electronics essentially rely on exciton diffusive dynamics that have to be controlled and observed to ensure the development of high-efficient organic devices.

Here we present a new technique based on ultrafast photoinduced absorption (PIA) spectroscopy that provides a direct handle on the exciton diffusion coefficient[1]. We applied the new method for real-time tracking of singlet exciton diffusion in vacuum-deposited layers of the well-known OSC acceptor, C_{70} fullerene. In our experiments, vacuum-deposited C_{70} layers of different thicknesses from 6 nm to 196 nm (absorber) are sandwiched between 10 nm thick layers of TPTPA which acts as a quencher and hole acceptor, with molecularly smooth interfaces (as tested by X-ray reflectometry). We demonstrate efficient singlet exciton harvesting from C_{70} layers up to 70 nm in thickness. The exciton diffusion process is temperature-independent down to 77 K, which implies extremely low energetic disorder of <5 meV. The experimental findings are excellently described by a simple analytical model and also supported by extensive Monte-Carlo simulations. The novel technique is deemed to pave the way to further development of efficient optoelectronic devices such as organic thin-film transistors, light-emitting transistors and lasers.

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Device physics of organic transistors

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Over recent years there has been tremendous progress in developing low-temperature, solution-processible organic semiconductors that provide high charge carrier mobilities for both n-type and p-type field-effect transistor operation, good operational stability and other functionalities such as efficient electroluminescene, sensing or memory functions. In this tutorial we will discuss the basic device and charge transport physics of organic transistors and will assess their performance in light of a range of applications in displays and integrated systems.

T-10

Charge-transfer states for organic solar cells, OLEDs and NIR photo-detectors

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Organic solar cells based on interfaces between electron donor and electron acceptor molecules have incident-photon-to-extracted-charge conversion yields of over 85%, and absorbed photon-to-extracted-charge conversion yields of 90-100%. Their power conversion efficiency is currently limited by their low operating voltage, as compared to the optical gap of the main absorber material, indicating large energy losses per absorbed photon. We explore possibilities for increasing the operating voltage and discuss the influence of the donor-acceptor interfacial area, electronic coupling and molecular reorganization. Charge transfer (CT) states at the donor-acceptor interface play hereby an important role. These states have interesting fundamental properties. Depending on the used donor and acceptor materials, CT states can be very emissive, or generate free carriers at high yield. The former can result in rather efficient OLEDs, via thermally activated delayed fluorescence. The latter property will be exploited to enable narrow band, near-IR photo-detection. This new type of photodetector competes in the near-infrared (NIR) wavelength range with standard organic photodetectors but extends their detection range to longer wavelengths.

T-11

Printed polymer and hybrid transistors: from fundamentals to high frequency devices

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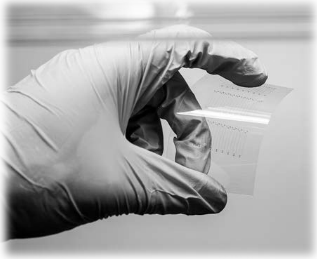
In this tutorial I will give an overview of fundamentals of organic field-effect transistors, then focusing on printed polymer devices. I will describe how it is possible to easily pattern all organic transistors and circuits through the use of only printing techniques, and how to achieve well-ordered and efficient charge-transport polymer nanostructures over large-areas. The level of control of the deposition process can boost the operational frequencies of printed polymer electronics well into the MHz regime without recurring to extreme downscaling, thus maintaining compatibility with cost-effective manufacturing of large-area circuits. A road-map to achieve GHz operation, thus enabling wireless data communication, within the context of a European project will be presented.



All-polymer, fully printed logic circuits @IIT.

Electrolyte-gated organic field effect transistors: fundamentals and applications to biosensing

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Organic field effect transistors (OFET) operated in aqueous environments are emerging as ultra-sensitive biosensors and transducers of electrical and electrochemical signals from a biological environment. Their applications range from detection of biomarkers in bodily fluids to implants for bidirectional communication with the central nervous system. They can be used in diagnostics, advanced treatments and theranostics. Several OFET layouts have been demonstrated to be effective in aqueous operations, which are distinguished either by their architecture or by the respective mechanism of doping by the ions in the electrolyte solution. In this work we discuss the chemical-physics of the electrolyte-gated OFET (EGOFET). We show how the substrate plays the role of a second bottom gate, whose potential is actually fixed by the pH/composition of the electrolyte and the gate voltage applied. The presence of the substrate can be exploited to modulate the capacitive coupling of the electrolyte solution with the semiconductor by almost one order of magnitude. We also show that this device, operated as a biosensor for a primary inflammatory citokine, i.e. TNF-alpha, responds super-exponentially in current vs analyte concentration in the sub-nM range, whereas responds linearly at concentrations greater than 1 nM. We unify the two regimes by introducing the density of states that is accessible upon the change of the electro-chemical potential of the organic semiconductor (pentacene) caused by the adsorption of TNF-alpha. We finally show that the response is modulated by the gate voltage applied, and the fit of the data allows us to extract the association binding constant of the antibody-antigen recognition, the molar free energy, and the electrostatic contribution to the free energy.

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T-13

Real Time X-Ray Studies of Organic Thin Films

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In the last years the surface sensitive X-ray techniques emerged to the versatile and frequently used methods in the field of the strutural characterization of thin films and patterned nanostructures. A combination of X-ray reflectivity (XR) and grazing incidence X-ray diffraction (GIXD), grazing incidence small-angle X-ray scattering (GISAXS) allow us to probe the ordering and structural properties along the surface normal as well as in the lateral directions.

Starting from general overview of the surface sensitive X-ray techniques; in the talk will be shown possible applications of these methods for the various classes of organic materials such as polymers and oligomers. The results of recent real time experiments performed at synchrotrons will be presented and a perspective of soft matter research with availability of novel nanobeam X-ray sources will be addressed. In particular, an advantage of nanodiffraction is to reveal a local orientation and to probe an interconnectivity of the conjugated network by X-ray cross-correlation analysis[1,2].

This work was supported by BMBF (project № 05K13PS4).

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Organic and Printed Electronics: Materials, Technologies, Opportunities and Challenges

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Organic and Printed Electronics are based on the general idea to use organic materials, formulate printing inks, and subsequently use these inks to print active electronic devices. Born approximately 10 years ago, the most prominent result of this idea are OLED displays as part of everyday smart phones and TV sets. Out of a total market of 23 Bn. US$, OLED represent the biggest share of 18 Bn. US$. Electrophoretic displays, also originating from this technology, have become the dominant display type for e-readers. However, 3rd generation solar cells, printed sensors and printed integrated smart systems are still in a waiting position to become mass products.

To provide electronic functions, basically three different types of materials are needed: semiconductors, conductors, and dielectrics. While the electronic properties of the classical semiconductor silicon can be tuned using elements such as boron and phosphorous, the molecular structures of organic semiconductors need to be precisely tailored to obtain the desired electronic properties. In addition, the deposition process significantly impacts the performance of the deposited film. Even though wet processed OLED were expected to have a clear cost, at present vacuum deposition still yields higher performing devices and allows a more robust manufacturing processes with higher yields. The lack of reliable wet processes was one of the factors delaying the further market acceptance of many organic and printed electronic components. To overcome this situation, the tool box for organic and printed components has been extended to inorganic materials, such as metal inks, classical patterning methods, such as lithography, and hybrids, devices combining printed elements with silicon-based chips. The choice and availability of materials and specific process technologies will be discussed for specific devices.

Invited lectures

I-1

Chemistry of Perovskite Solar Cells

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The discovery of inorganic and hybrid iodoplumbates with exciting photovoltaic properties has agitated a renewed interest in iodometallates. Started with only 3% of energy conversion efficiency in 2009[1], these compounds have quickly achieved an appreciable level of nearly 20% by the beginning of 2015[2] owing to the improved methods of preparation, doping, and cell assembling. However, besides various problems associated with their stability and scaling, iodoplumbates possess an intrinsic imperfection: they contain toxic lead, which is readily bio-available owing to the instant solubility of compounds in water[3]. In response to this issue, other iodometallates have become increasingly attractive, with tin, antimony and bismuth being the most explored metals[4]. In this paper, we discuss recent discoveries in the field of chemistry of iodoplumbate perovskite photovoltaics and provide insights into chemistry of alternative iodometallates and their potential as light-harvesting materials.

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I-2

Structural and electronic dynamics in hybrid perovskite materials for photovoltaic and light-emitting devices

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Organic-inorganic hybrid materials have recently attracted a lot of attention for optoelectronic applications as they allow for combining the flexibility and processibility of organic molecular systems with the good stability and charge-transport properties of inorganic crystalline materials.

In this contribution, we use ultrafast vis-pump / infrared(IR)-probe spectroscopy to investigate the optical signature of charge dynamics in CH3NH3PbI3 perovskite films. We observed that, in contrast to most inorganic semiconductors and quantum dot materials which demonstrate strong photoinducedn absorption in IR upon carrier generation, this perovskite show a complex response which involves strong ground-state bleach contribution. Such response is probably connected with the partial filling of intragap states next to the conduction band edge. It may also indicate the existence of Burstein–Moss type effect in perovskite materials.

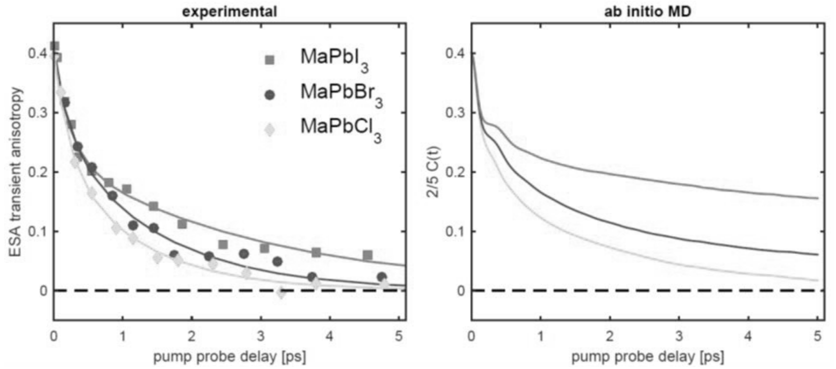

Fig. 1. a) Transient anisotropy dynamics of CH3NH3+ ion as measured in the centre of excited-state absorption (ESA) for NH3 bending mode. Dots show experimentally determined values for pure perovskites with different halide ions. (b) Rotational correlation function of MA as calculated based on ab initio molecular dynamics simulations for pure halide perovskites.

We also apply ultrafast two-dimensional vibrational spectroscopy and molecular dynamics simulations to elucidate orientational dynamics of organic methylammonium (CH3NH3) cation in a range[1] of pure and mixed tri-halide perovskite materials. For pure MAPbX3 (X=I,Br,Cl) perovskite films, we observe that cation dynamics slows down with increasing size and polarizability of the halide atom (Fig.1.). Much slower dynamics, up to partial immobilization of the organic cation, were observed in mixed CH3NH3Pb(ClxBr1-x)3 and CH3NH3Pb(BrxI1-x)3 alloys, which we associated with the symmetry breaking within the perovskite unit cell. The observed dynamics are essential for understanding the effects of structural and dynamical disorder in perovskite optoelectronic systems.

This work was supported by van Gogh grant from Dutch-French Academy.

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[1] A.A. Bakulin at al *J. Phys. Chem. Lett.*, 2015, ***6*** (18), pp 3663–3669

QM modeling of materials for organic electronics

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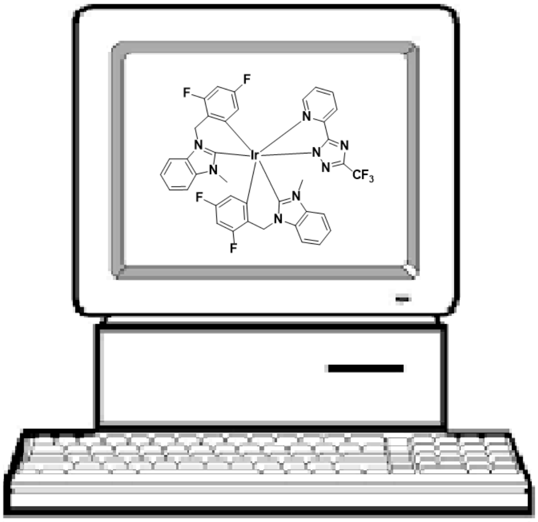
State of the art quantum-mechanical (QM) calculation methods enable predictive estimations of molecular properties at semi-quantitative level. This gives the opportunity to model various properties of organic molecules, such as geometry, electronic structure, and chemical reactivity.

This tutorial lecture will give basic information on how to use QM calculations in modeling of structure and properties of organic molecules relevant for applications in electronics. Examples of successful applications of QM calculations in the development of PhOLED, TADF, DSSC will be presented.



Spectroscopy of single conjugated polymers and aggregates

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A comprehensive understanding about the structure-photophysics correlations in conjugated polymers (CPs) is crucial for its development in optoelectronics. Unfortunately, this has remained elusive to date largely due to the macroscopic heterogeneity in both structural and photophysical properties of polymer materials. With single molecule/aggregate spectroscopy, we performed a systematic examination on the relationship between structure and important photophysical properties from single polymer chain up to bulk state.

Single polymer chain conformation was studied using polarization spectroscopy to examine how side-chains affect folding of the polymers. The effects of this folding are then correlated with differences in both single molecule spectra as well as transient "blinking". Aggregates of both MEH-PPV[1] as well as a variety of polythiophenes[2,3] were examined. Tunable interchain morphologies, i.e., packing order and distance, were achieved through altering the regioregularity and size of side-chains, respectively. Quantitative analysis on fluorescence transients suggested highly ordered interchain packing is in favor of long-range interchain energy migration, while disordered packing, even within just a few chains, can significantly impede the interchain mechanism. Beyond interchain disorder, the interchain electronic coupling can also be strongly inhibited by a long interchain packing distance and a competition from intrachain electronic coupling mechanism. In addition, the intrachain coupling was found to be enhanced as a result of increased backbone planarity, leading to the interchain mechanism overwhelmed and largely limited despite of short packing distance.

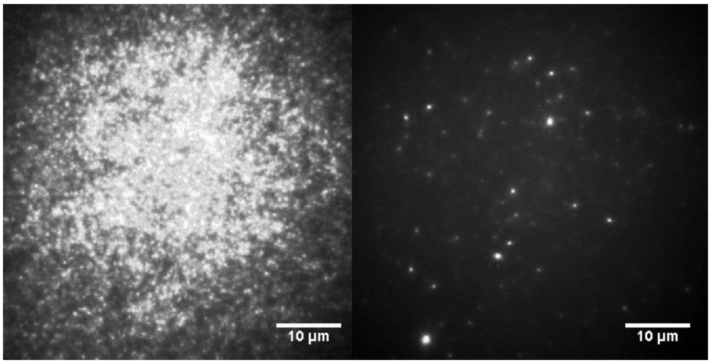

Figure 1: Single moleucle images of regioregular poly(3-hexylthiophene) before (left) and after (right) solvent vapor annealing to form small polymer aggregates

This work was supported by the US National Science Foundation(Grant CHE-1310222)

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I-5

Electron spectroscopy studies of organic electronics materials

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There is presented some background material on surface science approach to studies of the conjugated organic materials and organic thin film structures on solid surfaces. The mechanisms of the energy level alignment and the density of the electronic states at organic film interfaces with metal and semiconductor surfaces studied by core-level and ultraviolet photoelectron spectroscopy are considered. The electronic properties of the surface organic layers can be tuned by means of the influence of the substrate material and by introducing polar substituents into the molecules. Those changes may be readily monitored by the analysis of the density of valence states and on the density of the unoccupied electronic states (DOS and DOUS, respectively). Particular attention is paid to the techniques, which use the low-energy electron beam as a probe of the materials under study. Among them the total current spectroscopy (TCS) and dissociative electron attachment (DEA) are considered. Possible pathways for application of some recent results in electronics and medicine are presented.

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Russia's position in the emerging global industry of flexible electronics

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Keywords:

Flexible electronics, new electronics.

Abstract

Electronics is not only a driver for the development of computing power, but also a driver for the development of wireless networks. We live in a world covered by internet. Despite this, there still remains a large number of things around us that can potentially be linked through the internet. This will be possible when the technologies will reach the balance of three factors: the cost, the volume of production and the realization in any geometric form. Flexible and printed electronics are just such technologies. Applying the electronic identification on the packaging, stocks, retail products and on other objects, more and more information becomes available, which leads to the emergence of new services and business models. Beyond emerging possibilities of the identification, the new technology will introduce thin-film technology sensors and displays in the labels and patches. They will stimulate further development of the new services in the food security, counterfeit fight, advertising, healthcare and other areas. Confidently the new types of electronics - a flexible, organic, printed - is very fertile ground for the emergence of innovation in the near future.

In October 2015, the consortium of Russian nanotechnology centers established by Artek Electronics became an industrial partner of an affiliation program for the development of technology platforms in flexible thin film electronics by IMEC (Belgium). With the access to the latest technological solutions, the consortium begins to develop a broad range of applications based on flexible electronics for the transport and logistics, the retail and packaging, smart urban systems and infrastructures, personalized medicine and e-health.

The key goal of participation of the consortium of nanotechnology centers in the IMEC program on flexible electronics is a serial startup creation, developing products and providing engineering services in following applications:

- Transport and logistics (e.g. new generation of transport tickets with mini displays).
- Retail and packaging (e.g. food packaging with embedded sensors and indicators for food security).
- Personalized medicine (e.g. patches with sensors for pregnancy monitoring).
- E-health (e.g. car seats or mattresses for monitoring of key health condition parameters).
- New generation of urban infrastructures (e.g. smart highway with embedded RFID tags for collecting and transfer of road data to the automobile, increasing security of traffic and pedestrians).
- E-textiles (e.g. smart clothes for security services).

The key focus of the consortium is the development of the joint businesses in Russia with other industrial partners of the program – primarily due to the implementation of joint engineering and R&D projects for the creation and product customization for the Russian market.

Organic thin film transistors industrialisation and applications

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OTFTs (organic thin-film transistors) manufactured using low-temperature processes represent the lowest cost and most flexible platform for bringing any surfaces to life with displays and sensors. FlexEnable will present the latest performance of its OTFT technology, and its use in applications across consumer electronics, automotive, medical and security markets.

Harnessing Plasmonic Nanoparticles for Solar Cells

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The development of alternative sources of energy such as solar photovoltaic devices is one of the urgent problems of our society. In the field of photovoltaics (PV) the primary tasks are to increase the solar cells efficiency and significant reduction in their price. For the crystalline silicon solar cells, the problem of increasing their efficacy was largely solved, however they are still very expensive. By contrast, organic solar cells are rather cheap in production, but have quite low efficiency so far[1]. That is why the development of various methods that allows to increase the organic solar cells efficiency is of prime importance[2].

One option to raise an efficiency of a PV solar cell is the use of plasmonic nanoparticles, which are embedded into the solar cell. Each nanoparticle serves then as a nanoantenna allowing concentrating (guiding) the incident electromagnetic field in the absorption area and thereby increases the efficiency of the solar cell[3]. Such nanostructures are already used in silicon solar cells, but technologies of the nanostructure deposition are very expensive and laborious.

In this paper we review the recent progress in using plasmonic nanoparticles for improving the efficiency of the solar energy absorption in a PV solar cell with embedded plasmonic nanoparticles. Specifically, we will discuss how the nanoplasmonic particles can be used for guiding and concentrating the light for enhanced absorption, paying attention to both fundamentals and design considerations, as well as to realization of the broadband nanoplasmonic scattering to better utilize the incoming solar spectrum. Plus to that, we will discuss potential advantages of using dielectric nanoparticles in PV solar cells.

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Towards high performance organic semiconductor films on arbitrary substrates

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Keywords:

Organic semiconductors, organic semiconductor single-crystal growth, zone casting, organic transistor, mobility extraction, van der pauw.

Abstract:

In this presentation, we give an overview of our research efforts towards high performance organic electronics devices based on highly ordered thin films of organic semiconductors. The final goal is to realize high-performance electronic and opto-electronic organic devices such as transistors and light-emitting transistors. In the first part of the talk, we present methods to grow in a controlled way highly crystalline molecular layers on arbitrary substrates. In the second part of the talk, we provide a discussion on electrical characterization of high performance devices and present methods for a safe charge carrier mobility extraction.

We have developed several approaches to grow highly ordered films of organic semiconductors. The first method, applicable to small molecules, is based on evaporation through micron-sized shadow-mask openings. By reduction of the shadow-mask aperture size, nucleation in each opening is limited to exactly a single nucleus. A monolayer crystal with micron-sized dimensions grows from each single nucleus. We show the potential of the technique to form thin organic films with a controlled grain localization for the fabrication of thin films with known grain boundary density. A second method, applicable to soluble molecules, is based on zone casting. We have designed and built an apparatus in which the speed of the linear motion can be matched to the rate of solvent evaporation, between 25 and 200 µm/s. In this slow processing mode, we grow C_8BTBT films with a thickness of ~20 nm and with single crystalline domain size longer than 1mm. Transistors based on these films achieve excellent characteristics.

With their reduced channel resistivity, transistors based on high mobility organic semiconductors are quite sensitive to adverse effects from the contact resistance. Here we show that in frequent cases, contact resistance can give rise a serious overestimation of the semiconductor mobility when this parameter is extracted using the standard transconductance method. This counterintuitive effect arises when contact resistance shows a heavy non-linear dependence on the gate voltage. Better mobility extraction methods are desirable. One such method is the gated van der Pauw (gVDP) measurement. The gVDP device can be fabricated with simple methods and gives a stable and accurate measurement of organic semiconductor thin film mobility and threshold voltage that are independent of the resistance at the contacts.

This work is financed by grant # 320680 (EPOS CRYSTALLI) of the European Research Council.

I-10

Russian Flexible Electronics Centre – a platform for prototyping and small scale manufacturing

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Keywords:

Organic semiconductors, IGZO, organic transistor, facility

Abstract:

Nanotechnology center Technospark (Moscow, Troitsk) combine two thin-film transistor technologies based on metal-oxide and organic materials in one low-volume pilot-line facility in Troitsk. Russian Flexible Electronics Centre (RFEC) aims to establish a platform for prototyping and small volume manufacturing of new products based on flexible thin-film transistor technologies such as IGZO and oTFT. In partnership with leading European R&D companies imec (Belgium), Holst Centre, set up by imec and TNO (The Netherlands), and FlexEnable (Great Britain), RFEC will develop a range of advanced thin-film transistor technologies based on metal-oxide and organic materials. RFEC will focus on the customized development of new flexible electronics components (like displays, sensors, NFC and RFID tags) for end-user companies, high-quality prototyping and small volume manufacturing. Due to the close cooperation with global R&D leaders, RFEC has access to cutting-edge materials, equipment and processes. The established ecosystems of imec, Holst Centre and FlexEnable, including material and equipment suppliers as well as application and end-user companies etc. are an efficient vehicle to evaluate the upscaling of new technologies to volume manufacturing. Capacity of the plant is more than 5000m^2 of transistor matrix per year, that corresponds to 200 000 of 10” displays or more than 500 000 000 NFC tags.

Oral talks

O-1

Direct C–H Arylation Polymerization toward Sustainable Synthesis of Conjugated Polymers for High Performance Organic Electronics

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π-Conjugated polymers show great promise as lightweight, inexpensive, and earth-abundant materials for applications in organic electronics.[1] Direct C–H arylation (DAR) is a powerful tool for the synthesis of conjugated materials.[2] So far, DAR polymerizations (DARP) have had limited success at replacing traditional polymerization methods that employ pre-functionalized organometallic monomers (e.g., Stille and Suzuki polycondensations), especially for high-performing materials. We have developed a DARP method that enables the 'green chemistry' synthesis of a range of high performance low-bandgap polymers and demonstrated that they exhibit photovoltaic performance, optical properties, charge transport and recombination, and film morphologies that are comparable to those obtained via Stille polymerizations (Fig. 1).

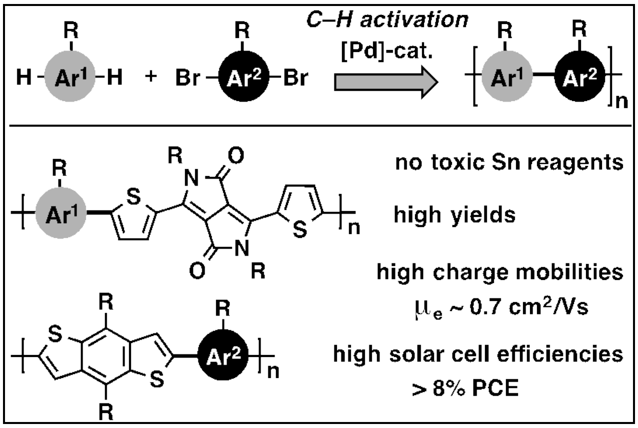

Fig. 1. Synthesis of π-conjugated polymers via DARP

The optimized DARP method affords conjugated polymers in excellent >90% yields with good-to-high molecular weights, having no apparent polymerization defects, and with photovoltaic performances exceeding 8%.[3] Full synthetic, mechanistic, and materials characterization details will be discussed.

This work was supported by Argonne-Northwestern Solar Energy Research (ANSER) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (Award Number DE-SC0001059).

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O-2

9*H*-Fluorene-9-ylidene-caped small molecules: toward rational design of conformational dependent optical properties for organic optoelectronics

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Highly emissive organic materials with external stimuli response like mechanical pressure, optical impulse or thermal annealing are of great importance for organic optoelectronic applications in light-emitting devices, functional sensors or security papers[1]. A design of organic molecules with desired absorption and emission features is a challenge task because several factors such as structure, crystal packing, the relative orientation of transition dipole moments etc. should be considered. By changing terminal substituents in linear π-conjugated systems different molecular packing can be achieved generating J- or H-aggregates with different intermolecular interactions and significant influence on emission properties[2]. In this work we synthesized and studied diphenylthiophene caped with fluorene groups - 2,5-bis(4-((9*H*-fluorene-9-ylidene)methyl)phenyl)thiophene (**BFPTh**, **Fig. 1**).

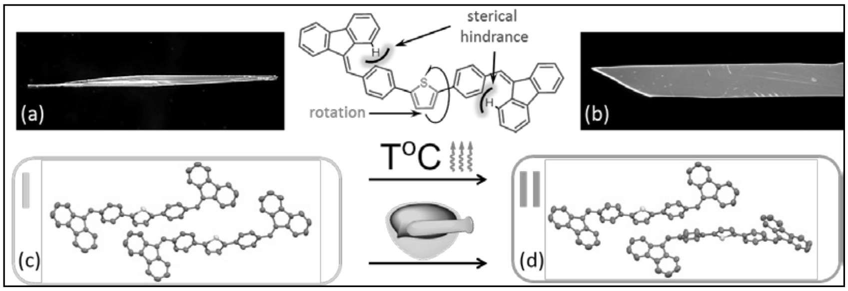

Fig. 1. Fluorescence mircographs of BPFTh single crystal polymorph **I** (a) and **II** (b); X-ray structure of dimers of polymorph **I** (c) and **II** (d).

The crystals of **BFPTh** have been grown by solvent-antisolvent crystallization. The crystals of the two conformational polymorphs with different emission color can be obtained selectively - triclinic orange needles **I (Fig. 1a, c)** or monoclinic green-yellow plates **II** (**Fig.1 b, d**). Photoluminescence quantum yield for both polymorphs reaches 31%. Polymorph **I** undergo mechano-(grinding) and thermo-responsive (~240°C) transformation to more therodynamically stable polymorph **II** that was confirmed by X-ray diffraction. It has been shown by TD DFT quantum chemical calculations that rotating of thiophene ring during transition of polymorph **I** to **II** led to dramatic change in electronic structure of the molecules resulting in changing of absorption and emission colours.

As a result of our study we suggest a rational design of highly fluorescent and thermo- or mechano-sensitive materials based on planar conjugated linker with bulky terminal groups having non-planar conformation.

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Design of donor-acceptor oligomers for solution-processed organic solar cells

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A library of donor-acceptor oligomers of linear[1-5] and star-shaped[5-15] architecture was designed and successfully synthesized (Fig.1). Systematic variations of the central donor units (cyclopentadithiophene, dithienosilole, dithienopyrrole, triphenylamine, tris(2-methoxyphenyl)amine), terminal acceptor groups (3-ethylrhodanine (alkyl-Rh), dicyanovinyl (DCV), alkyldicyanovinyl (alkyl-DCV), phenyldicyanovinyl (Ph-DCV)), lengths of either alkyl chain or oligothiophene π-bridge in the molecules allowed elucidating the structure-properties relationships in this series of molecules. Bulk heterojunction organic solar cells prepared from these molecules as donors and PCBM[70] as acceptor by solution processing showed power conversion efficiency up to 5.4 - 6.4%.

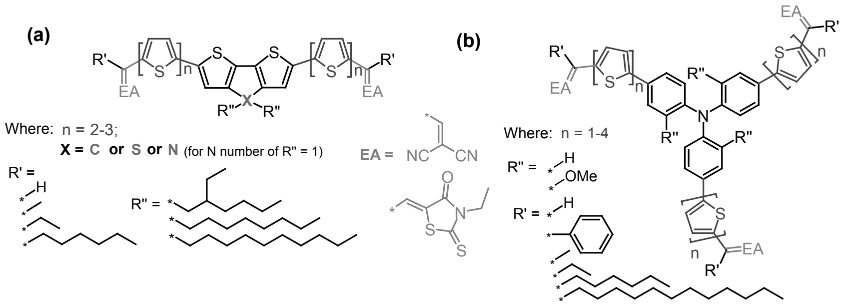

Fig. 1. Schematic representation of (a) linear and (b) star-shaped oligomers

The parts of this work including synthesis and characterization of linear oligomers with alkyl-DCV and alkyl-Rh were supported by RFBR (№15-33-20957) and Program of President of Russian Federation (MK-5061.2015.3), respectively. This work in the part of star-shaped oligomers was supported by Russian Science Foundation (14-13-01380).

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Nanostructured organosilicon luminophores – large scale synthesis and application in organic photonic and optoelectronic devices

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Organic luminophores are widely used to create advanced devices in different areas of science and industry like nuclear physics, photonics, medical diagnostics and so on. Above applications are highly demanding to spectral characteristics of active molecules. In particular, luminescence spectra of organic luminophores should cover the wavelength range from 300 to 700 nm. Additionally, absorption spectra must possess bands in a UV-Vis region (160-600 nm) with high extinction coefficient as $10^5 – 10^6$ L*mol*cm^{-1} and much more.

In ISPM RAS an approach to the synthesis of oligoarylsilanes consisting of several different luminescent fragments connected via silicon atoms has been developed[1]. This approach is very flexible and allows combining various functional fragments to obtain molecules with desired chemical structure and optical properties. The molecules synthesized possess unique properties: huge extinction coefficient, large Stocks shift and excellent luminescence quantum yield in a predefined spectral region, good solubility and processability that allowed to called them as nanostructured organosilicon luminophores (NOLs).[2,3]

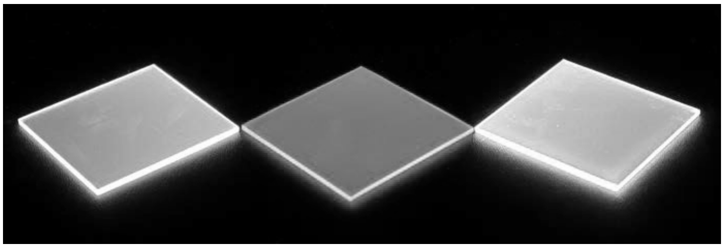

Figure 1. Photoes of NOL-containing PMMA plates under a UV irradiation.

In our innovative company LumInnoTech LLC we synthesize and upscale library of NOLs emitting in the whole spectral range (Figure 1). They can be used as effective spectral shifters in plastic scintillators and other radiation or elementary particles detectors[4], photodetectors, organic light emitting diodes and solar cells. Optical properties, solubility and phase behavior of NOLs can be flexibly tuned depending of the application requirements. We successfully developed a cost-efficient, low-waste technology of synthesis in pilot scale reactors. All luminophores synthesized are available for supply on demand in amount of hundreds grams.

This work was supported by Foundation for Assistance to Small Innovative Enterprises (Project № 21565).

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Resistive switches in composite structures based on organic dyes and colloidal nano plates CdSe

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Development of composite structures is an important direction in organic electronics. It was shown in our previous work that composite materials have high potential for memory applications[1]. Organic resistive memory is being widely studied due to its easy manufacture techniques and suitable operation parameters[2].

The operation principles of resistive memory presume an ability of the system to switch between at least two states "ON" and "OFF" with different resistances (resistive switches RS). Embedding metal particles (linear size ~5 μm) into isolating in pristine state polymer results in RS speed less than 15 ns, non-volatile characteristics, on/off ratio over 2 orders of magnitude, switching electric field below breakdown values, number of rewriting cycles 10^5 or higher[1]. Samples can be fully fabricated by printing techniques, and we demonstrated that there are no significant differences in their performance compared to samples on hard substrates[3].

For practical application further investigations of downsize scaling impact are required. Replacing metal micro particles with organic photoactive semiconductor particles of various sizes (1.3-2.3 nm in length and 0.3-0.8 nm height) allowed us to control switching voltage using external light source[4]. Introduction of inorganic nanoparticles (NP) can lead to increase in photoresponse and stability of RS in composite structures due to charge transport between NP and organic media. Moreover, energy levels of quantum size confinement in NP can provide photoactivation of RS at a certain wavelength that can be easily tuned by crystal size, form and chemical composition.

In this work we observed RS in composite structures consisting of polystyrene matrix with incorporation of colloidal nanoplates CdSe, *tert*-butyl-substituted lutetium diphthalocyanine, hexadecachloro-substituted lutetium triphthalocyanine and other dyes. We obtained similar results for coplanar and sandwich contact geometries. I-V curve in "OFF" state is attributed to Richardson-Schottky or Poole-Frenkel conduction mechanisms. In "ON" state I-V curve can be approximated by linear omic dependence, temperature dependence of conductivity demonstrates metallic type. RS is dependent on external illumination. Photoconductivity spectrum for composite structures demonstrates the same local maximums and minimums as absorption spectrum of NP that confirms charge transport between NP and organic media.

We demonstrated that incorporation of CdSe nanoplates into organic matrix provides a promising material for construction of high density and efficient memory.

This work was supported by RFBR (project № 16-07-00961, 15-03-05890, 16-33-60005).

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Selective mercury sensor model based on crown-substituted hemicyanine dye monolayer at air/water interface

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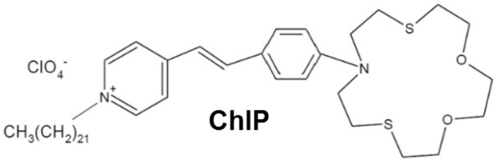
Hemicyanine dyes attract special attention due to their spectral characteristics and possibility to easily impart required properties to these compounds via chemical modification of terminal groups. In the present work, a hemicyanine dye was functionalized by dithio-aza-crown-ether group, which can selectively bind mercury ions, and an alkyl "tail", which provides amphiphility to the chromoionophore molecule (ChIP). Spectrophotometric and fluorometric titration of the ChIP solution by mercury perchlorate allowed us to register positions and intensities of absorbance and fluorescent emission bands of ChIP and its complex with mercury in solutions.



ChIP

Studies of the ChIP monolayers on aqueous subphases with different concentration of mercury ions by means of fiber optic reflection-absorption and fluorescence spectroscopy have shown that the studied chromoionophore forms complexes with Hg2+ at the air/water interface. However, in this case the structures of the complexes differ from ones in solutions due to the influence of interface, molecular surrounding, and surface pressure. This cation binding leads to a noticeable changes of dye monolayer absorbance spectra. Moreover, absorbance bands corresponding to complexes of 1:2 and 1:1 composition are observed depending on the concentration of the analyte in the aqueous subphase.

Structure and organization of the studied monolayers was also studied using grazing incidence X-ray diffraction and reflection. It is established that presence of barium cations in the subphase inhibits the head-to-tail aggregation of ChIP molecules in the compressed monolayer, which can be transferred onto solid substrate to produce a sensor element. This effect promotes such preorganization of the monolayer that significantly enhances efficiency of mercury ions binding by the compressed monolayer of studied chromoionophore due to crown-ether fragments of the molecules being more accessible to the analyte.

It is shown, that intensities of the ChIP monolayer emission peak obtained upon excitation at wavelengths corresponding to free-form dye (480 nm) and mercury complex (420 nm) depend on analyte concentration in the subphase. And ratio of their values can be used for convenient calibration curve for qualitative determination of mercury concentration in the aqueous medium. The advantage of the proposed approach is the presence of internal reference point in the system, analogous to one used in ratiometric sensory systems. It allows one to compare results obtained for films of different thickness, packing density and organization, since ratio between the intensities of the measured peaks is independent of these properties.

The study was supported by RFBR grants no. 16-33-60024 and 16-29-05272.

Multireference Quantum Chemistry in Organic Electronics

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The computational problems that typically arise in organic electronics are the problems of light absorption and emission, charge separation and recombination, and charge transport. These problems are usually addressed with the relatively cheap and fast density functional theory, which allows for large-scale calculations. However, this approach has intrinsic deficiencies that lead to qualitatively wrong results. Among these are overestimation of charge delocalization in extended molecular systems, underestimation of the energy of charge-transfer states, and different errors in the energies of singlet and triplet states, which lead to wrong transition probabilities of nonradiative processes.

Multireference methods, such as CASSCF/XMCQDPT, provide qualitatively correct and accurate description of the processes of interest. In particular, they correctly describe charge and exciton localization in extended systems through including the states with different localization with equal weights. They also provide balanced treatment of states of different multiplicity and different orbital character. Therefore, multireference methods give deeper insight into the nature of the systems under study. Understanding the mechanism of the target process will help one to find simple molecular descriptors that can be calculated by cheap methods in large scale.

We outline the problems in which multireference treatment is necessary, give some basics of the CASSCF and XMCQDPT methods, and demonstrate the application of multireference computational methods to the problems of light emission, charge and energy transfer, and chemical stability of typical OLED materials.

This work was supported by RSF (project № 14-43-00052).

O-8

Band-like transport and magnetic ions at organic charge transfer interfaces

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It has been shown that direct contact of two initially insulating organic single crystals can cause significant interfacial electrical conductance and in some cases can even lead to metallic behavior[1]. On the other hand, recent photoemission spectroscopy studies on film interfaces between two metal-organic molecules MnPc (Mn-phthalocyanine) and F_{16}CoPc (fluorinated Co-phthalocyanine) have detected a charge transfer with particular involvement of the transition metal centers of both molecules[2]. This results motivated us to investigate transport properties of charge transfer interfaces built with metal-organic magnetic molecules, expecting that the involvement of the metal ions into the charge transfer process might provide a good connection between magnetic and charge transport properties.

We have investigated an interface formed by a rubrene (tetraphenyltetracene) single crystal and F_{16}CoPc (fluorinated Co-phthalocyanine) film (Fig. 1a) by means of temperature dependent charge transport measurements, Hall effect, scanning Kelvin probe microscopy and photoelectron spectroscopy[3]. We have found that the charge transfer leads to significantly enhanced interfacial electrical conductivity and have determined the density, mobility and nature of charge carriers in the system (holes in rubrene, see Fig 1b). Moreover, we have found that the amount of charge transfer in F_{16}CoPc/rubrene is high enough to cause the band-like transport in rubrene crystals at the interface (Fig. 1c). Finally, our XPS and UPS measurements have shown that the charge transfer in F_{16}CoPc/rubrene involves electronic orbitals centered on the magnetic Co ions of the phthalocyanine molecules causing. Thus, F_{16}CoPc/rubrene is the first organic interface where the charge transfer responsible for the interfacial conductivity fully involves the metal Co core of the phthalocyanine molecules, providing a link between charge transport and magnetic properties.

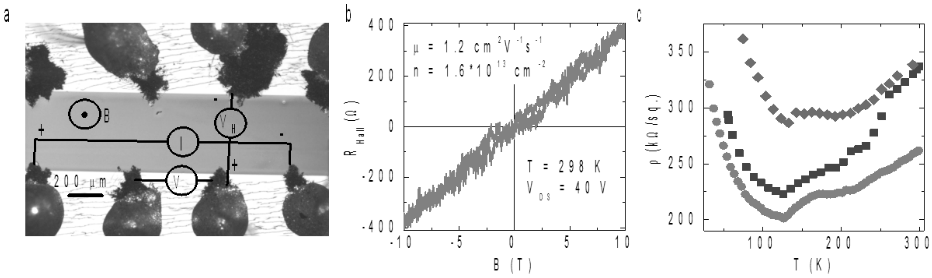

Figure 5. a) Optical microscope image of rubrene/F_{16}CoPc device. F_{16}CoPc film is evaporated on the surface of the rubrene crystal. **b)** Hall resistance vs. applied magnetic field measured for a rubrene/F_{16}CoPc device. **c)** Temperature dependence of the resistivity of three rubrene/F_{16}CoPc devices.

This work was supported by DFG (project № KR 4364/1-1 and KR 4364/2-1).

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O-9

Highly-emissive solution-grown furan/phenylene co-oligomer single crystals

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Materials combining high luminescence efficiency and charge transport are in strong demand for organic optoelectronics because of their potential applications in various light-emitting devices. Attainment of both these properties simultaneously possesses a great challenge because high mobility requires close molecular packing that usually leads to very weak emission[1]. One of the most useful routs for increasing luminescence is furan incorporation, which also yields an additional benefit of increased solubility highly favorable for industrial applications[2]. In this work, we demonstrate that solution-grown single crystals of furan/phenylene co-oligomer 1,4-bis(5-phenylfuran-2-yl)benzene (BPFB, Fig. 1a) combine high photoluminescence quantum yield (PL QY) with efficient charge transport.

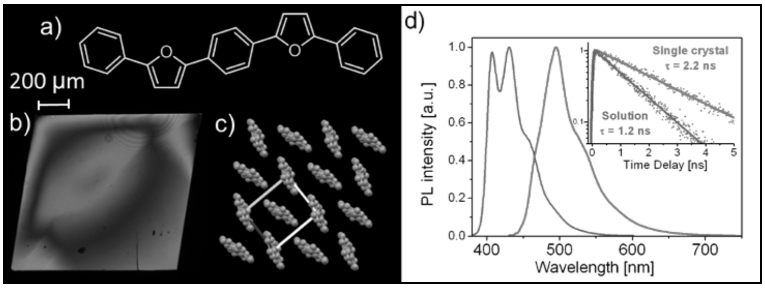

Fig. 1. a) Chemical formula of BPFB; b) Optical image of BPFB single crystal in transmitted light in crossed polarizers; c) Herringbone packing of BPFB molecules in the plane of the main crystal face; d) spectra and kinetics (inset) measured for diluted CH_3CN solution (olive) and single crystals (red).

Crystals were grown by solvent-antisolvent crystallization and had a rhombus shape (Fig. 1b). BPFB molecules are packed according to herringbone motif with the long molecular axis being almost perpendicular to the main crystal face. The crystals demonstrate hole mobility up to 0.1 cm^2/Vs and bright PL with PL QY exceeding 70% (reabsorption corrected). PL kinetics (Fig. 1d) are monoexponential and show that close packing of BPFB molecules in single crystals increases the PL lifetime by a factor of ~2. Our data suggest that high luminescent properties of BPFB single crystals stem from their highly ordered and low-defect structure. Such a combination of high PL QY with good charge transport properties demonstrates that solution-processable furan-phenylene single crystals are promising materials for organic optoelectronics.

This work was supported by RFBR (project 16-33-60011) and RSF (project 15-12-30031).

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O-10

Dopant-enhanced photoluminescence in solution processed semiconducting single crystals

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Organic semiconducting crystals can combine efficient charge transport and high luminescence[1] allowing fabrication of high-performance organic optoelectronic devices such as light-emitting transistors and lasers. One of the promising approach to enhance the luminescence properties of organic semiconducting crystals is doping by highly luminescent molecules.[2] If the absorption spectrum of the dopant overlaps with the fluorescence spectrum of the host material, the host-dopant energy transfer can improve the luminescent properties of the material. Earlier the dopant-enhanced luminescence was demonstrated for a vapor-grown organic semiconducting crystals,[2] whereas doping of solution-processed crystals is more advantageous for organic electronics printing technologies.

In this work, we demonstrate that the photoluminescent (PL) properties of organic semiconducting single crystals are enhanced by controlled doping via solution processing. As the host material we used thiophene-phenylene co-oligomer (TPCO) 5,5'-bis(4-(trimethylsilyl)phenyl)-2,2'-bithiophene (TMS-PTTP-TMS) as it demonstrated a promising combination of high PL and efficient charge transport.[3] As a dopant, a longer TPCO 5,5'''-bis(4-(trimethylsilyl)phenyl)-2,2':5',2'':5'',2'''-quaterthiophene (TMS-PTTTTP-TMS) was used as its absorption spectrum overlaps with the PL spectrum of the TMS-PTTP-TMS (Fig. 1a).

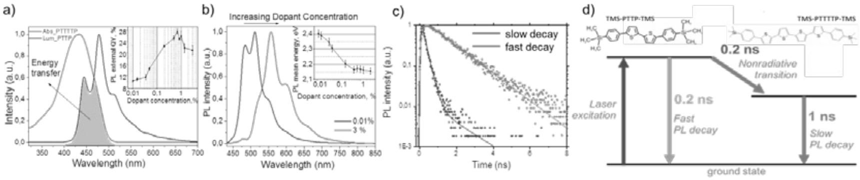

Fig.1.(a) PL spectrum of host and absorption spectrum of dopant in solution; the inset shows PL external QY for single crystals as a function of dopant molar concentration; (b) PL spectra of 0.01% and 3% doped single crystals; the inset shows the PL mean energy as a function of dopant concentration; (c) PL decays for the blue (485 nm) and red (590 nm) spectral components in the doped crystal; (d) energy diagram of the doped crystal with characteristic time constants from the kinetic model.

We observed that the PL spectra shift to the red upon increasing the dopant concentration (Fig.1b). Time-resolved PL data (Fig.1c) show that the red part of PL is delayed and decays longer as compared to the blue part. These PL dynamic features indicate efficient host-dopant energy transfer (Fig.1d), with the dopant molar concentration 0.7% providing the maximum value of PL quantum external yield (QY) (inset in Fig.1a). We conclude that doping of organic semiconducting single crystals by a highly luminescent dopant via solution processing is a promising route for designing the novel organic optoelectronic materials compatible with printing technologies of devices.

The work is supported by Russian Science Foundation # 15-12-30031.

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Thiophene-phenylene co-oligomer single crystals unintentionally doped by longer co-oligomers: optical and electrical properties

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Thiophene-phenylene co-oligomers (TPCO) single crystals are promising materials for organic light emitting transistors (OLETs) and injection lasers as they combine high luminescence yield with efficient charge transport.[1] However, the nature of excellent luminescent properties of TPCO single crystals have not yet been properly understood.

In this work, we demonstrate that luminescent properties of 4-5-ring TPCO can be dominated by impurities that are longer TPCO unintentionally appeared during the synthesis. Trying different synthetic routes to TPCO having the conjugated core PTTP and PTPTP (P and T are phenylene and thiophene rings, respectively) with various end groups (H, F, CF_3, trimethylsilyl), we have identified the presence of longer TPCOs at a concentration less than 1%. The TPCO crystals were grown from the vapor phase and from solution.

We have found that the photoluminescence (PL) spectrum and quantum efficiency (QE) of the TPCO single crystals are strongly varied with the concentration of longer TPCO, as they have a lower bandgap energy. These dopants act as an excitation energy funnel (Fig.1a) usually increasing the PL QE in some cases even higher than that of the diluted solution. Surprisingly, the unintentional doping did not show any noticeable effect on the hole mobility so that is beneficial for OLETs. The crystal growth via physical vapor phase transport (PVT) technique (Fig. 1b) was found to decrease the impurity concentration in the TPCO crystals. Fig.1c shows that the crystals distributed along the growth zones have significantly different PL spectrum and QE. The solution growth methods resulted in TPCO crystals containing the amount of impurities similar to the initial material (powder).

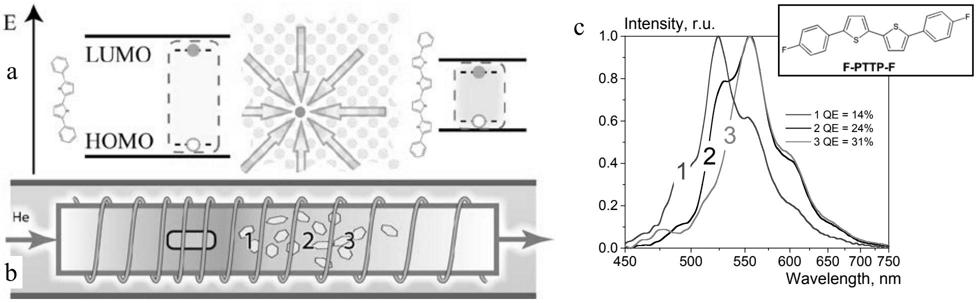

Fig. 1. a) Schematic of energy funneling from host TPCO to dopants; b) PVT growth setup, 1,2,3 denote growth zones; c) PL spectra of crystals grown in zones 1,2,3.

We conclude that TPCO doping by longer co-oligomers is a promising route to more efficient optoelectronic materials and devices converting electricity to light.

This work was supported by RFBR (project № 15-02-09375), Russian Science Foundation (project № 15-12-30031) and Lomonosov MSU Program of Development.

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Mono- and tri-methine carbocyanine dye J-aggregates: Influence of aggregation promoters on optical and stability properties

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Nanoscale-ordered supramolecular particles possess optical, electric, emission characteristics which significantly exceed those of molecular material. One of the examples of self-assembling followed by the substantial change of physical characteristics is cyanine (polymethine) dye aggregation called J-agregation[1]. Recently our group showed successful fabrication of optoelectronic switches based on single-ribbon[2] (Fig.1) and multi-layer[3] cyanine dye J-aggregates. However, there still remained the unsolved issue of the device limited stability due to degradation and photobleaching in the visible light.

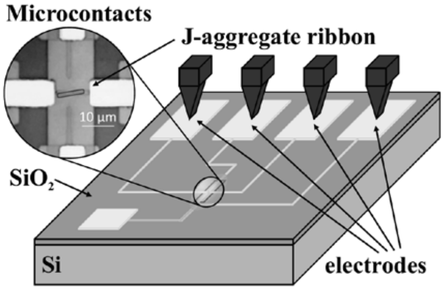

Fig. 1. Microstructure with single J-aggregate ribbon performing as optoelectronic switch

In this paper we investigate the influence of 4 additives, PDAC polycation electrolyte and salts of Na, Mg, Eu, on J-aggregates of 4 slightly different carbocyanine dyes formation in aqueous solutions with the emphasis on dyes' optical properties changes and stability. Studied optical properties include separated D-,M-,J-peaks analysis – extinction ratio, peak FWHM, central wavelength etc. Respective properties were studied via spectrophotometry and atomic force microscopy techniques (for dye degradation in films). Studies indicate the peculiarities of each dye, showing mono-methine thiacarbocyanine (MMTC) to be sensitive to all additives studied, tri-methine thiacarbocyanine – mainly to Na and Mg salts, tri-methine oxacarbocyanine – insensitive to all additives utilized. Eu is shown to easily hinder further aggregation of all studied dyes, with the formation of colloid at large concentrations. PDAC also acts quite selectively – mainly aggregating MMTC instead of other dyes, and also in large concentration forming a colloid with dye. These facts are quite interesting and demonstrate that question of organic crystal stabilization[4] is highly complicated and depends on various factors such as ionic strength of stabilizing agents and dyes, pH of solution, solvation, etc. and needs to be carefully investigated in the framework of organic single molecular devices development.

This work was supported by Russian Science Foundation under Grant No. 14-19-01308.

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O-13

Current trends in Spectroscopic Imaging Ellipsometry and Brewster Angle Microscopy

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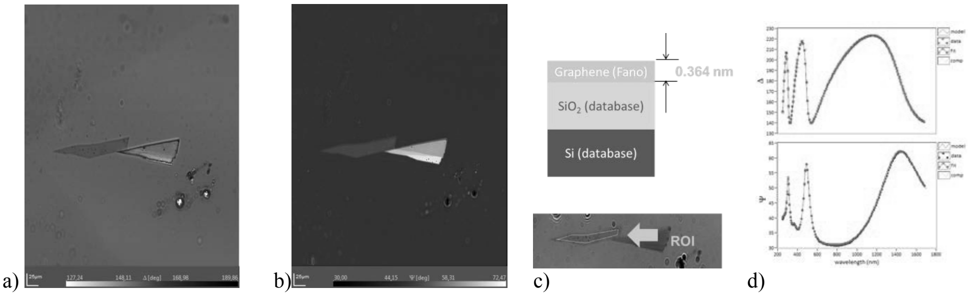
Conventional ellipsometry is well established in the field of thin film metrology due to the exceptionally high resolution in the z-axis, enabling very accurate thickness measurements for nano- and microfilms. However, conventional ellipsometry does not have a sufficient lateral resolution for a number of the described developments nor a direct microscopic visualization with highest contrast. The approach of spectroscopic imaging ellipsometry (SIE) differs from conventional ellipsometry in that the measurements are based on a series of micrographs taken at dedicated orientations of the optical components. The primary measurements are microscopic maps of the ellipsometric angles Delta and Psi (Fig. 1 a, b) or micro maps of dedicated elements of the Müller Matrix. Areas can be condensed by binning, averaging of selected pixels data (Region of interest, ROI) of equivalent areas and by using histogram data of inhomogeneous regions.



a) b) c) d)

Fig. 1. Spectroscopic imaging ellipsometric measurement of a Graphene flake: Delta (a) and Psi (b) map – examples of a graphene flake, selected Region of Interest and Optical model (c) and wavelength spectra of Delta and Psi, (d) extracted for the ROI from Delta and Psi maps recorded for wavelengths in between 250 and 1700 nm (measured points and model, line).

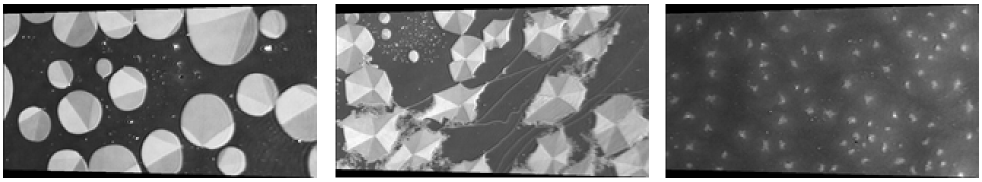


Fig. 2. Micrographs, recorded with a Brewsterangle Microscope with modified Scheimflug optics (Ultrabam, Accurion, Germany).

Brewster angle microscopy is the preferential method for the mesoscopic characterization of monolayers at the air interface without a transfer to a solid substrate. The “trick” is based on the fact that at the Brewster angle of incidence a parallel polarized laser beam has zero reflectance and the image is black. But even after tiny impacts to the refractive index like a domain of a condensed monolayer, the Brewster law is not fullfilled anymore. The surface is reflecting light and by using a high intensity light source like a laser, nanofilms can be imaged directly on the water surface. The talk will include an introduction to both techniques and dedicated examples of applications.

O-14

Enhanced Exciton Harvesting in Rubrene:C$_{60}$ Heterojunctions

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In organic solar cells (OSCs), separated charges are generated via dissociation of the photogenerated excitons at the interface between donor- and acceptor-type materials. In majority of donor/acceptor combinations, only singlet excitons are harvested, while the triplet excitons do not contribute to the OSC photocurrent. However, the diffusion length of triplet excitons is typically much longer compared to singlets. Furthermore, in many organic materials extremely efficient singlet-to-triplet conversion occurs that limits singlet exciton lifetime and hence the diffusion length. Therefore, utilization of the triplet excitons is one of the routes to increased charge generation in triplet-populated OSCs.

Here we use time-resolved photoluminescence (PL) to track the exciton dynamics in amorphous and crystalline rubrene layers of rubrene/C$_{60}$ planar heterojunctions. We show that in both crystalline and amorphous rubrene fast singlet fission (SF) occurs populating the rubrene layer with triplet excitons. The dynamics of the triplets are tracked by delayed PL caused by triplet-triplet annihilation (TTA) events. In the amorphous system, dramatic quenching of prompt singlet PL is observed in rubrene/C$_{60}$ bilayer, while delayed PL dynamics are unchanged (Fig. 1a). Therefore, only singlet excitons undergo dissociation at the *amorphous* rubrene/C$_{60}$ interface, while the triplet excitons cannot be harvested. This is in sharp contrast with the *crystalline* samples, where delayed PL dynamics are noticeably different in the bilayer because the triplet excitons dissociate at the interface, Fig 1b. The process of triplet exciton dissociation is possible due to the significantly lower energy of the interfacial charge transfer (CT) state in *crystalline* rubrene/C$_{60}$ samples as compared to the *amorphous* ones, as obtained from sensitive external quantum efficiency measurements[1]. This, together with the extremely fast fission process, makes crystalline rubrene-based devices essentially triplet-driven.

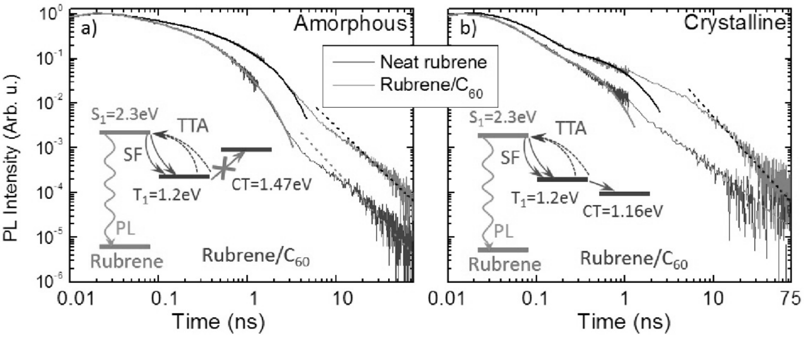

Fig. 1 Log-log plots of PL dynamics and energy diagrams[1] for amorphous (a) and crystalline (b) rubrene samples. The experimental data are shown by the red (neat samples) and blue (C$_{60}$-paired samples) thin lines. The multiexponential fits of early-time decays are shown by thick lines, while the linear fits at longer times are shown by the dashed lines.

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[1] YunHui L. Lin *et al.*, submitted.

Water – based processing of electro-active layers in organic solar cells

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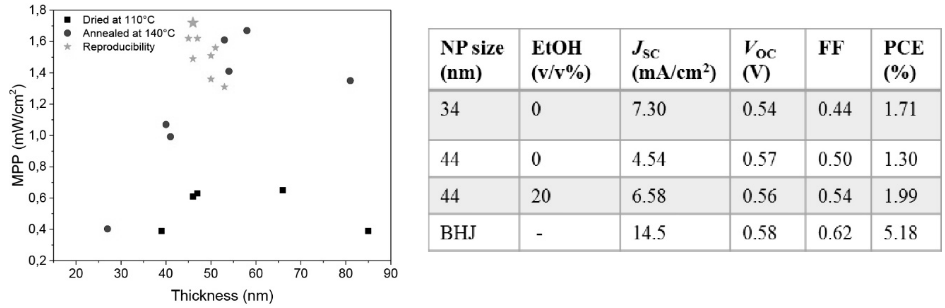
Over the past few years, the PCE of OPVs dramatically increased due to a great development of new donor polymer materials having improved charge carrier mobility and energy alignments. An emerging field of research is the development of new acceptor materials with tuned energy alignments and broad absorption spectra in the visible light with promising PCEs exceeding 10%. However, the vast majority of record efficiency solar cells have been obtained by processing from chlorinated solvents which are harmfull for health and environment. An eco-frienly alternative is necessary to promote the large scale fabrication, where water would be most favorable. OPV materials can be processed from water by precipitation on the nanometer scale in the presence of a surfactant. A drawback of this method might be charge recombination or inefficient charge transport induced by the ionic surfactant in the active layer. In this work we show that with careful optimization of the synthesis process eco-friendly solar cells can be made from a DPP polymer with [60]PCBM where the surfactant can be efficiently removed from the active layer.



NP size (nm)	EtOH (v/v%)	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	PCE (%)
34	0	7.30	0.54	0.44	1.71
44	0	4.54	0.57	0.50	1.30
44	20	6.58	0.56	0.54	1.99
BHJ	-	14.5	0.58	0.62	5.18

Fig. 1. (Left) influence of annealing on solar cell performance with different active layer thickness, (right) overview of performances with different NP size compared to a BHJ

After spin-coating the dispersion on an electron transport layer, water is removed from the film followed by an annealing step resulting in a continuous film of merged NPs. In order to obtain reproducible solar cells the surfactant concentration needs to be optimized, which has been done by dialysis, since too much surfactant causes de-wetted films while too less causes aggregation and rough active layers. Efficiencies exceeding 1.5% could be obtained with a reasonable reproducibility, as can be seen in the left image of Fig. 1. AFM studies have showed that the ionic surfactant diffuses to the solid-air interface while drying, after which it can be efficiently removed by a washing step. Therefore it is most likely that the low FF of these devices is not caused by the surfactant but caused by the morphology. By tuning the NP size the morphology can be altered which interestingly affects the device performance. Studies to the phase separation within the NP is therefore in progress and essential to obtain more insight to the active layer morphology. Additionally, addition of ethanol to the dispersion decreases the surface tension and enhances the *J*SC of the devices, caused by a higher contribution of the polymer to the photocurrent (see Fig. 1, right). A promising efficiency up to 2% could be obtained after optimization of the NP synthesis, however, especially due to the low *J*SC, the performance does not compete yet with a BHJ. Further research is in progress to understand the current limitations of these NP based solar cells.

O-16

The effect of branching in a semiconducting polymer on the efficiency of organic photovoltaic cells

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In the field of organic solar cells, conjugated polymers with a push-pull design have extensively been developed for use as electron donors in the active layer of these devices. Most of these polymers have a simple, linear architecture of the conjugated backbone implanted with alkyl chains to ensure solubility in organic solvents. In this work, the effect of a branched structure of the conjugated backbone on the physical and photovoltaic properties is investigated. It is found that branching has a dramatic effect on the solubility of these polymers, forcing the use of only 1% of branching moieties in the polymer. Uv-vis absorption and HOMO and LUMO energy levels of the branched and linear polymers are very similar, however a difference in aggregation strength is noted.

This difference in aggregation has a strong effect on the morphology of the active layer upon spin coating: in both cases a fibrous network of polymer is obtained, but the size of these fibres differs greatly. The branched polymer consistently shows finer fibrous structures than the linear one. This has a large effect on the photovoltaic efficiency of these layers, in particular on the short circuit current density, which increases upon branching. This eventually leads to an improvement of the power conversion efficiency of 4.4% for the best device of the linear polymer, to 6.3% for the best device of the branched polymer. (see fig. 1)

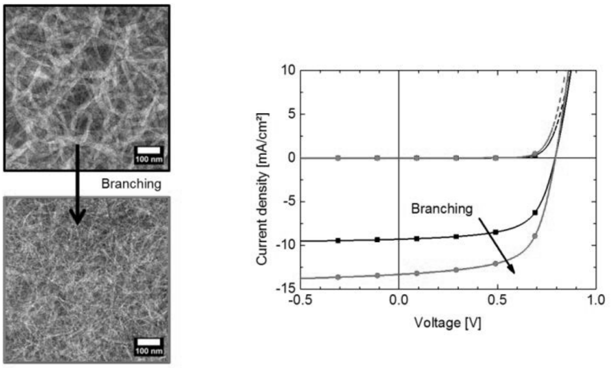

Fig. 1: The effect of branching on morphology and solar cell performance.

Further research into the morphology formation is conducted by *in-situ* light scattering experiments during spin coating. These experiments eventually lead to the assertion that the branched polymer has a lower barrier for nucleation, owing to its molecular structure, resulting in the formation of smaller fibres. This result is consistent with the difference in solubility.

This work was supported by the Agency for Innovation by Science and Technology in Flanders.

O-17

Structure-property relationships for bis-diketopyrrolopyrrole molecules in organic photovoltaics

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While diketopyrrolopyrrole (DPP) polymer photovoltaic materials have achieved power conversion efficiency (PCE) above 8%[1,2], the design of small molecules for efficient solution-processed organic solar cells is hampered by the absence of relationships that connect molecular structure via processing to blend morphology and power conversion efficiency. Moreover, the well-defined chemical structure and mature purification process make small-molecule materials more suitable for industrialization. Here we study a series of bis-diketopyrrolopyrrole (bis-DPP) molecules in which we systematically vary the aromatic core, the solubilizing side chains, and the end groups to achieve power conversion efficiencies of 4.4%. By comparing the morphology and performance we attempt to identify and rationalize the structure-property relationships. We find that the tendency to aggregate or crystallize are important factors to control and that these require a subtle balance.

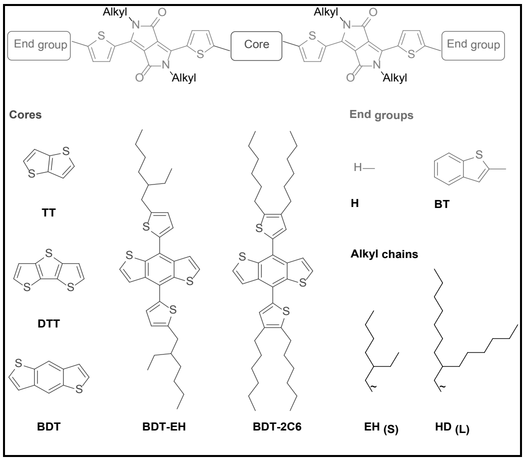

Fig. 1. Structures of Bis-DPP molecules.

The choice of co-solvent and thermal annealing condition has also been studied. For these bis-DPP molecules with fused aromatic cores, 1-chloronaphthalene (1-CN) plays a positive role in morphology after spin coating. Thermal annealing improves the efficiency of molecules with moderate aggregation and crystallization tendency. With these results, some structural factors for designing successful bis-DPP small molecules for solution-processed organic solar cells emerge. Solubility and tendency to crystallize are important to achieve the small domain size (10-20 nm) which is necessary for a good performance. Yet, strong effects are seen with subtle changes and, hence, evolutionary rather than de novo design of successful molecules will remain the most likely option to progress in this field for some time.

This research forms part of the research program of the Dutch Polymer Institute (DPI), project #762. Dutch Polymer Institute (DPI), P.O. Box 902, 5600 AX Eindhoven, the Netherlands.

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O-18

Stepwise change of conjugated polymer:acceptor blend properties with acceptor electron affinity

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Blends of conjugated polymers with small-molecule acceptors are widely used as active layers of organic solar cells. The blend morphology is of high importance for the device performance and is strongly dependent on the interplay between the donor-donor, acceptor-acceptor and donor-acceptor interactions. Some conjugated polymers form charge transfer complexes (CTCs) with small-molecule acceptors modifying donor-acceptor interaction[1]. CTCs can be inherited from solution into the film resulting in dramatic changes in the film photophysics[2]. However, a systematical study of the role of the donor-acceptor charge-transfer interaction in the blend morphology was not performed yet.

In this work, we address the effect of the donor-acceptor interaction on the film morphology and photophysics for blends of model conjugated polymer MEH-PPV with electron acceptors of the fluorene series. The donor-acceptor interaction was tuned by varying the acceptor electron affinity (EA), since CTC is stronger for higher EA. We observed a stepwise morphology change when the acceptor EA exceeds a threshold value. Specifically, the X-ray diffraction data (Fig. 1a,b) indicate an abrupt crossover from the segregated polymer and acceptor phases for the blends with low EA (< 3.7 eV) acceptors to the semicrystalline intermixed structure for the blends with high EA (> 3.7 eV) acceptors. According to Raman spectroscopy data (Fig. 1b, black dots), this crossover is accompanied by a stepwise increase in ground-state charge transfer for high-EA acceptors. Similar stepwise behavior was observed in polymer photoluminescence quenching (Fig. 1b, blue triangles) showing the close relation between the morphology and photophysics. To explain our data, we propose a morphological model based on the Flory-Huggins theory.

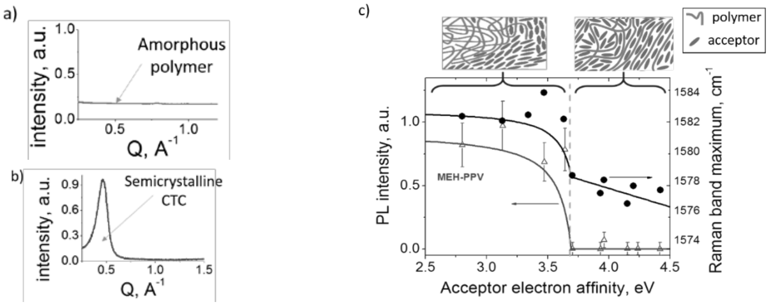

Fig. 1. Changes in properties of MEH-PPV:fluorene acceptor films with acceptor EA. X-ray diffraction data for the blends with low-EA (a) and high-EA (b) acceptors. (c) Photoluminescence intensity (blue) and frequency of the strongest MEH-PPV Raman band (1582 cm^{-1}) (black) as a function of EA. Insets illustrate the morphology of the blend.

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Structure of star-shaped D–π–A oligothiophenes in solid state and in thin films

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Recent progress in the field of bulk heterojunction and organic solar cells shows strong connection of power conversion efficiency to molecular packing of small molecules in solid state and in thin films[1,2]. Since type of crystal and mesophase ordering varies greatly on structure of branched oligothiophenes, optimizing core, length of thiophene block and functional groups provides demanded molecular design. Current contribution will describe such variations with triphenylamine (TPA), TPA-OMe$_3$ and 9-phenylcarbazole-based cores, 1T to 3T thiophene blocks and different alkyl, ethylrhodanine or phenyl end-groups and corresponding changes in their thermal and structural behavior.

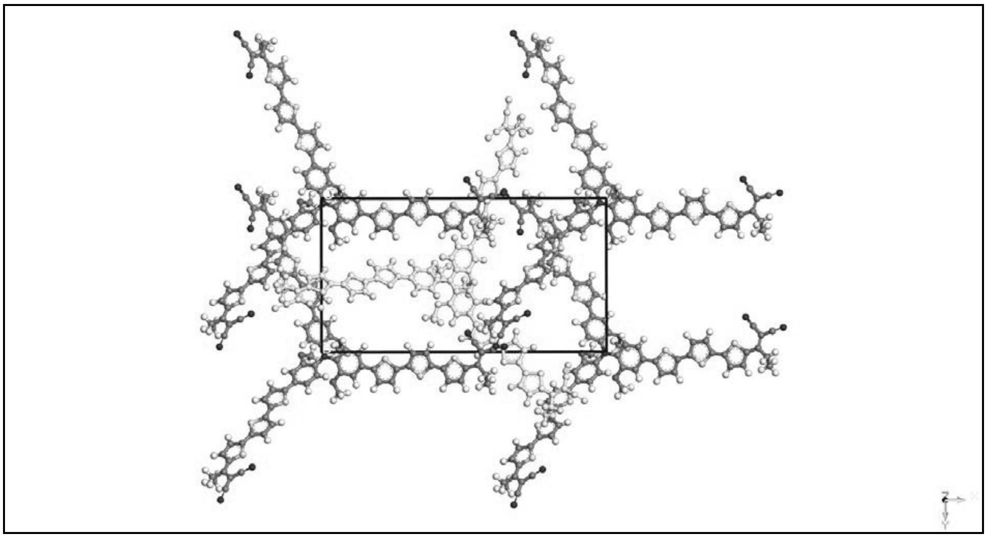

Fig. 1. Example of crystal cell packing for N(Ph-OMe- 3T-DCV- Et) 3

By means of X-ray diffraction in small and wide angles phase behavior was studied for a large series of novel star-shaped oligothiophenes using synchrotron radiation at Kurchatov Institute, ESRF and DESY. The type of organization differs from amorphous state to single-crystal with even a small change in molecular design. Furthermore, structure of pristine and blended with C70 oligothiophene thin films was investigated by grazing X-ray diffraction and reflectivity. Thus, a connection of structural ordering to the functional effectivity will be derived.

This work was supported by RFBR (project № 15-33-70055).

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O-20

Towards high performance organic –inorganic perovskite photovoltaics with CNT based top electrode

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Keywords:

Perovskite, single wall carbon nanotubes, SWCNT, organic –inorganic photovoltaics, printable electrodes, SWCNT nano-inks.

Abstract:

In this presentation, we give an overview of our research efforts towards investigation of new nano-ink materials for creating industrial methods of processing perovskite photovoltaic devices.

One of major technological limitations of perovskite processing is the problem of top electrode made by evaporation of gold in vacuum. Such a method is expensive and limits a time of processing. For industrial applications new materials for replacement of gold should be investigated.

In the framework of Solliance Perovskite and Organic Photovoltaics research program on the developing of perovskite photovoltaics industrial processing methods, the set of samples of nano inks was tested at imec. Solartek, as industrial partner of Solliance has provided samples of nano-inks and dry SWCNT for producing nano-ink at imec. Water-based CNT ink, Glycerol-based CNT ink and ODCB-based CNT ink were tested.

The possibility to deposit CNT-based inks via spray coating, to form top electrode by air drying has confirmed for water-based and ODCB-based inks.

Water-based CNT ink is good for spray coating to form top electrodes with thickness from 600nm to 5 µm. Up to 13.1% PCE has obtained. After 75 hours at RH 77% samples formed from water based CNT were more stable than referent sample with gold electrode. The efficiency of devices with CNTs and Au is practically the same after 550 h of illumination under 1 sun, but the degradation processes are different.

Drivers of the development of organic electronics as a framework for the applied laboratory

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Keywords:

Organic electronics, applications, market and technology drivers.

Abstract:

In this presentation, we give an overview of the main drivers for the development of the sector of organic electronics

Organic electronics represent a highly promising technology and a fast growing market. As a promising technology organic electronics has a lot of advantages.

The market for organic electronics could enjoy a compound annual growth rate (CAGR) of 29.5% between now and 2020, propelling the industry to a global worth of $79.5 billion. A commonly known application of organic materials is organic light-emitting diode (OLED), Organic solar cells, television displays, and transistors. Potential applications of organic electronics span a broad range of fields including national security, environmental health, biomedical research and IT. Some of the innovative applications of organic electronics appears in the field of embedded smart electronic systems.

Beside new applications, the main drivers of the market growth are expected to be technological advancements concerning organic display technology, developments in organic photovoltaics, transistor technology and organic polymer materials.

At present, disadvantages of organic electronics development include high cost on research &development activity. Increased spending in R&D will help accelerate the sector's deployment and improve efficiencies and cost. Recently established IFMO University laboratory of organic photovoltaics and electronics aims to establish a platform effective research and development to localize and accelerate the development of these sector in Russia.

Flexible and Organic Electronics developments at LG Group of companies

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In this talk I will describe the recent developments in the field of flexible and organic electronics in LG Holding, including LG Electronics, LG Display and LG Chem companies. This includes the research and development on flexible OLEDs, flexible solar cells, flexible touchscreens, flexible batteries etc.

I will report on all stages of flexible electronics development: from materials and components towards the single devices and further circuits and products.

Since LG is a conglomerate of companies, all materials for flexible electronics are made in-house. This starts actually from the substrates, the most up to date is research on high temperature stable transparent polyimide substrates, which stay the temperature high enough for LTPS (low temperature polysilicon) deposition and sintering, next one in the row it the barrier layers, which are important components of Flexible Electronics. A number of barrier layer types, developed will be discussed. OLED structures require not only barrier layers, but also special sealants and getter layers, which also were developed in house. Then come the materials themselves – including OLED materials, Organic PV materials organic TFT materials, battery materials. Although the structures are confidential, I will report about trends in the areas mentioned.

Next come devices and I will describe flexible backplane TFT panel concepts, as are seen by LG Display, I will also describe typical OLED structure, especially soluble OLED ones, which are last coming and finish with flexible battery types and structures.

As for devices a number of flexible concepts are under development or produced by LG. I will describe the concept of wearable devices as it is seen by LG now, also describe flexible smartphone concept and describe some in detail about automotive applications of flexible electronics, starting from morph type OLED lighting, conformable displays, windshield electronics, flexible sensors and touchscreens and will talk about printed electronics in EV and HEV.

In the last part of my talk I will report about application of flexible electronics in IoT (Internet of Things), including flexible RF-ID and antennas, flexible signage for Intellectual Shopping, flexible circuits to make IoT solutions cheaper and Smart Home solutions will be mentioned.

Coming from circuits to appliances I will share the vision of LG of how the flexible solutions can change consumer goods and make new market opportunities, especially pointing healthcare solutions, medical devices and wearables markets.

The future vision of LG on flexible electronics will be reported, with the accent made on 2D materials as a basis for next generation devices and organic materials viable for some applications. The next trend as printing with nanoparticle based inks and the application of nanoparticles in real devices will be considered

Finally the market of flexible electronics and it's perspectives as seen by LG Company will be reported.

Poster presentations

P-1

Ambipolar transport in single crystal field-effect transistors based on thiophene-phenylene co-oligomers

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Ambipolar organic field-effect transistors (OFETs) are necessary for multifunctional electronics, e.g. to fabricate integrated circuits with lower power dissipation and higher robustness[1]. Moreover, ambipolar charge transport is necessary for light-emitting transistors, which can have higher emission efficiencies compared to the light emitting diodes[2]. Among various types of ambipolar OFETs, single crystal devices based on thiophene-phenylene co-oligomers (TPCOs) show the best performance combining high charge mobilities and large luminescence quantum yield, so they are very attractive for applications in light-emitting field-effect transistors (LEFETs). TPCO single crystals formed by TMS-PTTP-TMS (Fig.1) combine high photoluminescence quantum yield (PL QY) exceeding 50% with charge mobilities up to 0.1 cm^2/Vs.[3]

In this work, ambipolar transport in OFETs based on TMS-PTTP-TMS single crystals is studied. TMS-PTTP-TMS crystals were grown using physical vapor transport (PVT) technique. Devices were made on highly doped silicon wafer with a 300-nm-thick SiO_2 layer, which was coated with a 30-nm-thick PMMA layer to remove electron traps on the SiO_2 surface. The shadow effect was used for thermal metal co-evaporation to attain asymmetrical source-drain electrodes, device structure is shown on Fig.1. We have measured the hole mobility 0.1 cm^2/Vs in the unipolar regime with symmetrical gold electrodes and 6*10^{-4} cm^2/Vs for both holes and electrons in the ambipolar regime with asymmetrical ytterbium-gold electrodes. Fig. 1 shows transfer characteristics in the ambipolar regime. The transistors show almost symmetrical transfer curves due to similar mobilities and close threshold voltages for electrons and holes that together are good for emitting area positioning. We compare devices with different crystal thicknesses and discuss the ways to decrease the threshold voltage and enhance the ambipolar transport.

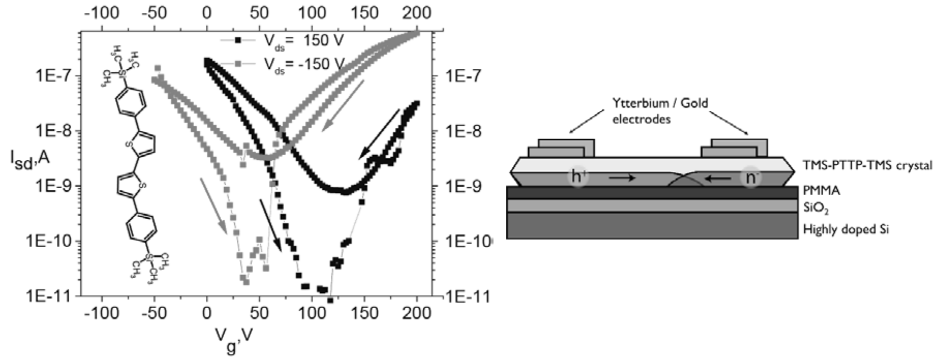

Fig. 1 Transfer characteristics of ambipolar OFET, chemical structure of TMS-PTTP-TMS and device schematic structure

This work was supported by Russian Science Foundation, #15-12-30031

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New chromophores based on combination of thiophene, ethylenedioxythiophene and carbazole fragments: synthesis and optoelectronic properties

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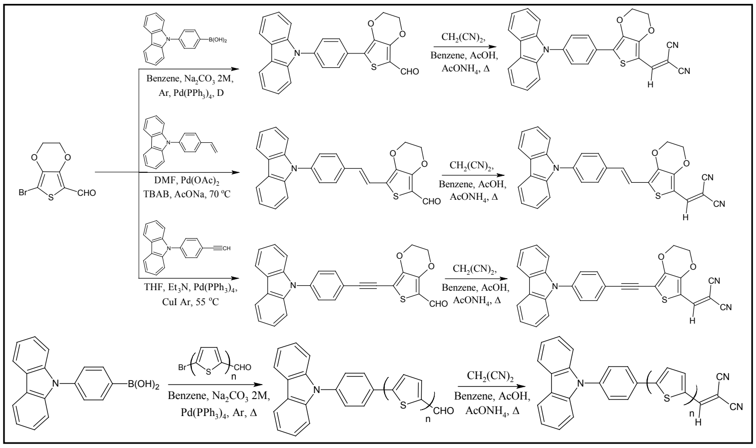
Organic π-conjugated materials constituted as various combination of different aromatic carbo- and heterocyclic electron donors (A) and electron acceptors (D) are of great interest from the point of view of their application in construction of optoelectronic devices such as organic field-effect transistors, organic photovoltaics, and organic light emitting diodes[1]. Variation of D and A moieties allows to tune HOMO and LUMO levels, and, as the result, the band gap values. Introducing into the structure of these compounds such powerful electron excessive heterocyclic fragments as thiophene and especially 3,4-ethilendioxythiophene allows to extend the absorption spectrum due to the intermolecular charge transfer from donor to acceptor[2]. This work presents the synthesis and investigation of D-π-A structures including 2,2-dicyanoethylene as electron acceptor group. Carbazole, thiophene and 3,4-ethilendioxythiophene were built into the structures of prepared compounds as electron donating fragments. In order to prepare the target compounds we have used such palladium catalyzed reaction as Suzuki, Heck and Sonogashira couplings.



Electronic absorption and fluorescence spectra were obtained for all the synthesized compounds. Electrochemical properties of compounds were investigated as well with the help of the cyclic voltammetry. The surface morphology of prepared films were studied by scanning tunneling microscope NTegro – Prima

The work was financially supported by the Ministry of Education and Science of the RF (project N 012011461916) and by RFBR (projects N 14-03-00341a, 14-03-96003_Ural-a). Instrumental studies were performed with the help of equipment purchased at the expense of the Program of National Research Universities of RF (Perm State University).

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Electroluminescent polynorbonenes with pendant ionic iridium(III) complexes as perspective emitters for OLEDs

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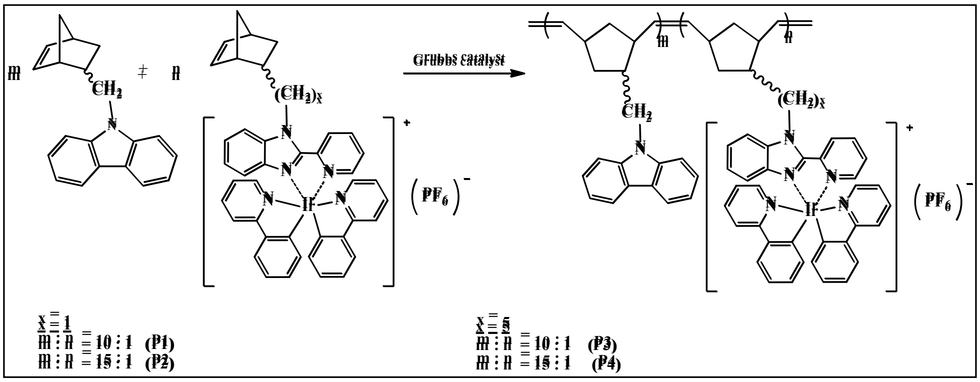
Functionalized polynorbonenes with luminescent ionic iridium(III) complexes in side chains were prepared by Ring-Opening-Metathesis Polymerization:



To investigate the electroluminescent properties of copolymers P1 – P4, OLEDs with the structure of ITO/Ir-copolymer/BATH/AlQ$_3$/Yb were fabricated.

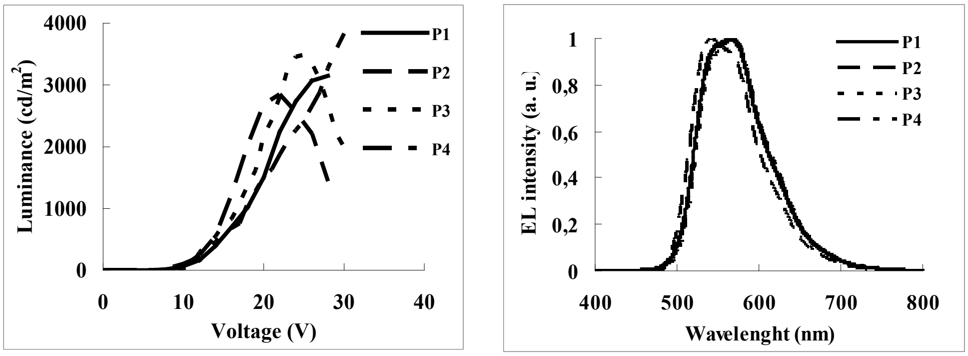


Fig. 1. Brightness-voltage curves and electroluminescence spectra of OLEDs using P1 – P4 as emitters

The devices produced yellow light. Maximum brightness of 3830 cd/m^2 and current efficiency of 36.8 cd/A were reached.

This work was supported by the RFBR (project No 15-43-02178-r_povolzh`e_a)

P-4

A Single Crystalline Organic Semiconductor with Mechanochromic and Solvatochrmic Properties and Facile Metal Coordination

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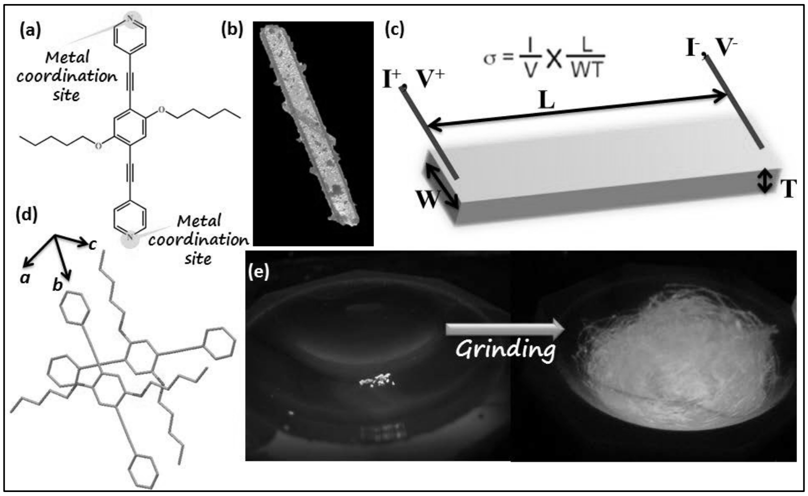
The use of small-molecule organic semiconductors in electronic devices has increased rapidly over the past decade. These molecules have caught the fancy of researchers globally since they are easy to synthesize, can be crystallized and deposited easily by solution and evaporation techniques, and have also very high mobilities. Herein we report the synthesis of an *oligo*-(*p*-phenylene) ethynelene (OPE) based novel organic molecule **1**. The compound yields highly emissive light green needle shaped crystals when crystallized by a vapour diffusion method.

From Single crystal X-ray diffraction, it is found that the molecules pack in a unique staggered morphology, imparting symmetry, which indicates electron transport and conductivity through all the faces of the crystal. True to our predictions, **1** shows a good semiconducting property with the conductivity obtained from the single crystal being $1.62x10^{-5}$ S.m^{-1}. **1** has metal coordination sites in the form of pyridinic nitrogens, and can be assembled to for Metal-organic frameworks (MOFs) with enhanced conductivity. Also, the compound shows mechanochrmoic and solvatochromic properties.



(a) Compound **1** **(b)** The single crystal of **1** **(c)** Conductivity measurement from the single crystal of **1** **(d)** Molecular packing in the crystal of **1** **(e)** Mechanochromism in **1**

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Nanostructured organosilicon luminophores for organic optoelectronics

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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 at 1-2 nm distance necessary for efficient Förster energy transfer.[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. 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).[7]

We applied NOLs as spectral shifters in new highly effective plastic scintillators (radiation detectors). Since two different luminophores are fixed properly on the nanoscale distance at the same branching molecule, both the light output and the attenuation length of the plastic scintillators significantly increase. This lead to a new type of scintillating devices with nanostructured luminophores[1]. Heat treatment of the NOLs and organosilicon oligomers having reactive vinyl and the hydride groups in solution, allowed to obtain transparent fluorescent organosiloxane composites stable over a wide temperature range[8]. The new NOLs used in various devices of organic photonics and electronics, such as spectral shifting fibers, organic light-emitting diodes (OLEDs)[9], CIGS photovoltaic devices[10].

NOLs are commercialized by a startup Limited Liability Company "Luminescent Innovative Technologies" (LumInnoTech LLC). All the details can be found on www.luminnotech.com.

Synthesis of amorphous NOLs was supported by Russian Science Foundation (grant 15-12-30031). Synthesis of model linear benzothiadiazole-based oligomers supported by Foundation of President of the Russian Federation (project MK 6501.2015.3).

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P-6

In pursuit of high efficiency hybrid devices: Functionalization of Gallium nitride surfaces

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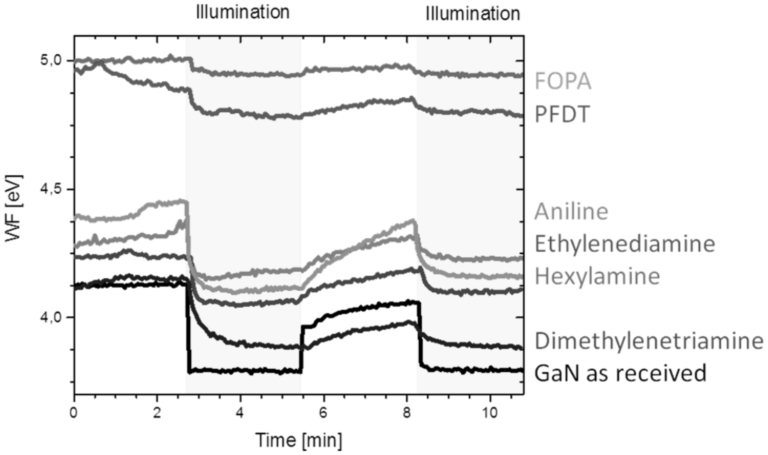

Fig. 1: Response of the surface work function of GaN(0001) to above band-gap UV-light illumination for different organic surface modifiers.

Gallium nitride (GaN) is an often used III-V direct band-gap semiconductor due to its excellent optoelectronic properties. GaN nanowires with different doping domains have become a promising candidate for efficient blue LEDs. Nevertheless, GaN suffers from a photoluminescence quenching effect, which previous works attributed solely to surface states[1]. In order to passivate those surface states the surfaces are modified with different self-assembled monolayers (SAMs), such as amines, thiols and phosphonates from solution. Wet chemically etched n-type GaN (0001) surfaces are compared electronically and chemically with adsorbate functionalized surfaces by atomic force microscopy, ambient Kelvin probe, XPS, UV-Vis spectroscopy and goniometry. We show that a thin surface layer which is desorbed under UV-irradiation in UHV is connected to the non-radiative recombination on the surface. Special attention is given to the difference observed between XPS and ambient Kelvin probe (KP) work function (WF) measurements in response to illumination as shown in figure 1 for KP. The reduction of the surface potential was previously falsely attributed to band bending[2]. However it has to be stressed that an X-ray induced SPV is possible. Modification of the surface with SAMs tuned the absolute WF as well as the light induced shift of the surface potential from 350 meV to as low as 80 meV.

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P-7

Thiophene-phenylene co-oligomer single crystals: effect of end groups

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Single crystals of thiophene-phenylene co-oligomers (TPCO) are promising optoelectronic materials for light-emitting devices as they combine efficient charge carrier transport and high luminescence[1,2] [1,2]. These electronic properties are controlled by the chemical structure of the molecules and their crystal packing; however, the structure-property relationships in TPCO single crystals have not yet been properly understood. For example, the TPCO single crystals show a considerable effect of end molecular groups on the crystal packing[3] [3] that is expected to affect the charge transport and optical properties.

Here, we study the impact of molecular end-groups on the properties of TPCO single crystals among 5 TPCO with the same phenylene-thiophene-thiophene-phenylene (PTTP) conjugated core (Fig. 1a, left).

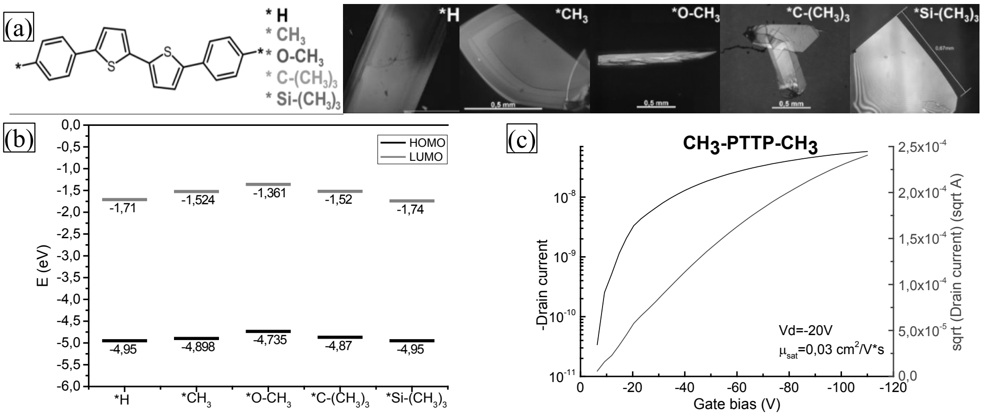

Fig.1. a) Chemical structure of TPCO and microscopy images of crystals, b) HOMO and LUMO energy levels of TPCO calculated using DFT method with 6-31g* basis set, c) transfer characteristics of CH_3-PTTP-CH_3 single crystal OFET in the top-contact bottom-gate geometry.

Calculated HOMO and LUMO energy levels of the TPCOs (Fig.1b) show their small variation (<0.22 eV) with the end-group type. Therefore, one can expect very similar charge injection conditions for all the TPCO. Single crystals of TPCO derivatives were grown using physical vapor transport technique (Fig. 1a). Variation of the end-group types results in a significant impact on the crystal shape. We fabricated single-crystal OFETs in top-contact bottom-gate (silicon oxide dielectric) and top-contact top-gate (parylene dielectric) geometries with printed and vacuum-deposited electrodes. Figure 1c shows a typical transfer characteristic for CH_3-PTTP-CH_3 single crystal as an example. All the five types of single crystals exhibited p-type semiconductor behavior with charge carrier mobility in the range 0.03–0.1 cm^2/Vs indicating similar charge transport properties. We conclude that although various end-groups affect the crystal structure, they do not influence significantly on charge transport properties.

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P-8

TCTA based single-molecular organic field effect transistors with single-walled carbon nanotubes contacts

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The ability to control of the conductance of single molecules will have a major impact in nanoscale electronics. Understanding of the electron transport in atomic and molecular scale nanodevices can be achieved from the formation of molecular junctions. However, it is a big challenge to control the type and quantity of molecules in the channel and the impact of the contacts. I-V characteristics dependence on temperature can help to distinguish between pristine contacts resistance and molecules and to determine the type and number of molecules. Single-walled carbon nanotubes (SWCNTs) (provided by Professor A. Nasibulin, Skoltech) were deposited on Si/SiO_2 substrate using gas-phase process formation based on thermal decomposition of ferrocene in the presence of carbon monoxide. Source and drain 100/5 nm Au/V electrodes were fabricated by photolithography, the gate electrode was high doped (p^{++}) Si substrate. Using focused ion beam we cut SWCNTs between 2 μm gold contacts and made gaps of 20-40 nm. Tris(4-carbazoyl-9-ylphenyl)amine (TCTA) molecules were deposited onto nanotubes and in the gaps between SWCNTs using physical vapor deposition. After the deposition three types of structures were made: pristine SWCNT FET, SWCNT covered with TCTA molecules and OFET with TCTA channel and SWCNTs contacts. The morphological, optical as well as I-V characteristics at different temperatures of fabricated FET devices were measured.

We produced OFET devices based on 20 nm TCTA molecular channel with linear mobility as high as 28 $cm^2/(V\cdot s)$. The transfer I-V curves and hysteresis behavior, measured at different temperatures, provide insight about the conductivity nature. We found that for pristine nanotubes the hysteresis loop tends to decrease its FWHM due to trap states in SiO_2 and adsorbate rearrangement near the channel, when the temperature is increased, while for covered nanotubes and molecules in the channel the dominant mechanism is charge impurities, which diffuse into the channel after applying the gate voltage. The transfer I-V curves for covered SWCNTs show a two step behavior with a plateau, which indicates that two types of materials are involved in the transport.

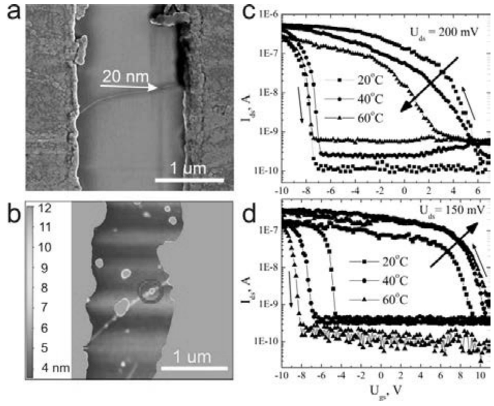

Figure 1. (a) SEM image after SWCNT cutting, (b) AFM image after TCTA molecules deposition, (c,d) transfer I-V curves for pristine SWCNT (c) and for TCTA channel (d)

This work was supported by RSF (grant №14-19-01308).

Correlating low-and high-frequency vibrations of a thiophene-phenelyene co-oliogemer single crystal with its lattice parameters

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Organic light-emitting field-effect transistors (OLETs) allow creating bright and flexible displays that can be more efficient and convenient than modern OLED displays. Single crystals of thiophene-phenelyne co-oligomers (TPCOs) are appropriate candidates for OLETs owing to their high luminescence and effective charge transport. However, in TPCO single crystals the correlation of the molecular order with charge transport and light emission properties is practically unexplored[1].

In this work, we study crystal structure, low- (LF) and high-frequency (HF) vibrations of TPCO 5,5′-bis[4-(trifluoromethyl)phenyl-1-yl]-2,2′-bithiophene[2] (CF_3-PTTP-CF_3). According to the X-ray diffraction analysis, its crystals have only 2 molecules per unit cell that simplifies the analysis of the crystal structure role in charge transport and thus in OLET performance.

We have recorded HF and LF Raman spectra of solution, powder and single crystals and explored anisotropic properties of scattering. Optical characteristics and intramolecular vibrations were calculated using density functional theory (DFT). The DFT results correlate well with the experimental data (fig. 1a). LF Raman spectra are of particular interest as this part of the vibrational spectrum (~10-200 cm^{-1}) enables us to study collective vibrations of the crystal lattice. By studying the temperature dependence of the LF Raman spectra (fig. 1b), we correlate the vibrational force constants with the crystal structure parameters extracted from the X-ray diffraction data recorded at different temperatures (fig. 1c). The interrelation between intermolecular packing, vibrations and semiconducting properties of the studied crystals are discussed.

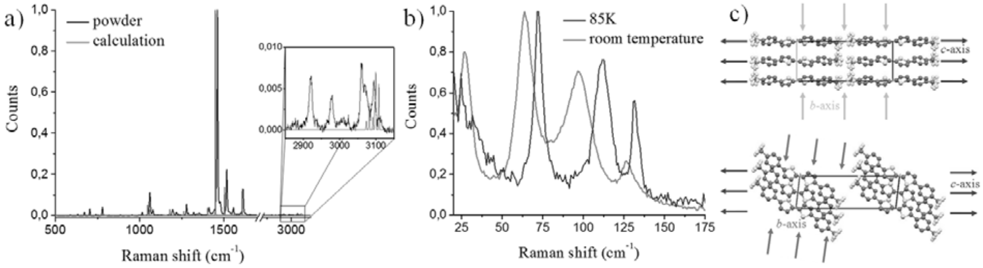

Fig. 1. a) Experimental and calculated HF Raman spectra; b) LF Raman spectra for different temperatures; c) projections of CF_3-PTTP-CF_3 unit cell with directions of deformation under cooling.

This work was supported by RFBR (project № 15-02-09375).

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P-10

Synthesis and physico-chemical properties of 1,4-bis(5-arylfuran-2-yl)benzenes

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α-Oligofurans has been shown to be perspective materials for organic electronics applications[1]. Compared to thiophene analogs, furan containing compounds demonstrate higher rigidity, higher solid state fluorescence and solubility and comparable semiconducting properties. Also, they potentially can be obtained from renewable sources and are considered to be biodegradable[2]. Moreover furan/phenylene co-oligomers recently have been shown to have efficient luminescent properties, ambipolar charge transport and application in organic light-emitting transistors[3].

In this work we have synthesized and studied novel alternating furan/phenylene co-oligomer 1,4-bis(5-phenylfuran-2-yl)benzene (**BPFBs**) and its methyl-substituted derivative (Fig. 1).

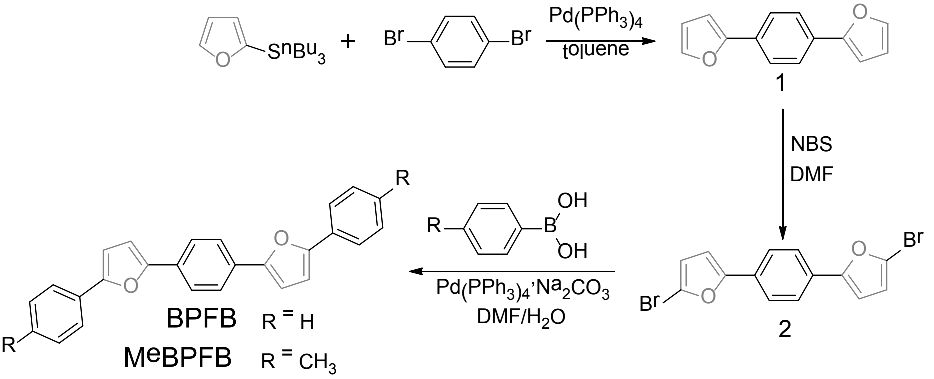

Figure 1. Synthesis of BPFB and Me-BPFB

BPFB derivatives were obtained by the combination of Stille and Suzuki cross-coupling reactions (Fig. 1.). Cyclic voltammetry measurements reveals that BPFB have first reversible oxidation peak that means that it is stable upon multiple Red/Ox cycles which is highly favorable for charge transport. The thermal stability was investigated by TGA and DSC analysis. BPFB has been shown to be stable at inert atmosphere and do not show any signatures of decomposition up to melting point (>238°C) at oxidizing atmosphere. The photostability in solution and solid state is also discussed.

The introduction of terminal methyl groups into BPFB has been shown to dramatically change the properties and reduce solubility. The crystal structure has also been shown to change due to tilting of the molecules.

This work was supported by RFBR (project 16-33-60011).

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Large-Area Ultrathin Single Crystal Films as an Active Layer for Organic FETs

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Organic field effect transistors (OFETs) based on single crystals provide the best performance comparable to one for a-Si devices[1]. However, single crystals are usually grown as free-standing samples, which should be transferred on an OFET substrate, or, for macro-crystals, be used without it in the top-gate OFET geometry. Withal we know that charge transport in OFET occurs in a few molecular layers close to the dielectric[2], hence the single crystals for OFET can be ultrathin. For organic electronics printing technologies, growth methods of ultrathin single-crystal films from solution directly on substrates are in strong demand.

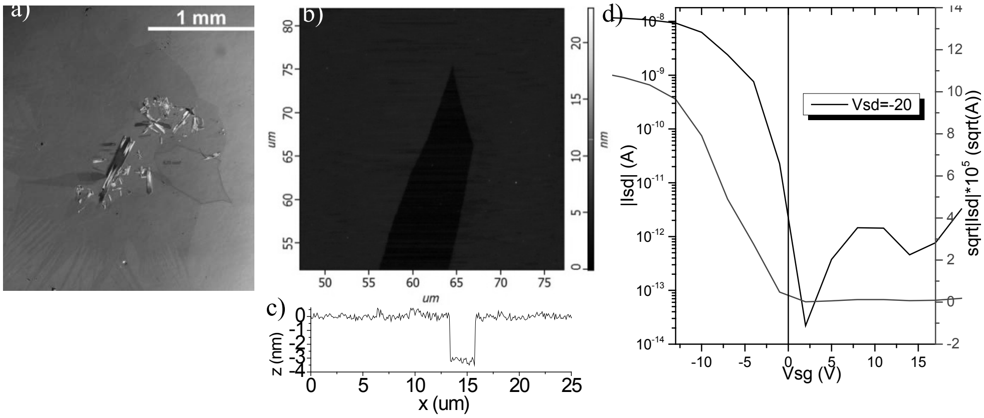

Fig. 1. DH-TTPTT thin films and OFET data. (a) Optical image; (b) AFM image of two crystalline domains jointing; (c) the corresponding surface profile; (d) OFET transfer curves.

In this work, we present a novel method of growing ultrathin single crystal films directly on substrates and demonstrate OFETs based on these films. As a semiconducting material, we used thiophene-phenylene co-oligomer 1,4-bis(5'-hexyl-[2,2'-bitiophene]-5-il)benzene (DH-TTPTT). Single crystal films were fabricated directly on the Si substrate with SiO_2/PMMA gate dielectric by spin-coating of DH-TTPTT solution in dichlorobenzene and further annealing in closed Petri dish. Single crystal domains, which were identified by polarization optical microscopy, typically have linear dimensions of 150–500 um with a thickness as small as 3 nm (fig. 1a-c). The films were used as an active layer for OFET with microprinted PEDOT:PSS top electrodes and SiO_2/PMMA as a gate dielectric. The OFETs demonstrated hole mobilities up to $1.2\text{x}10^{-2}$ cm^2/Vs with zero threshold and I_{on}/I_{off} as high as 10^5 (fig 1d). The OFET performance is among the best reported for monolayer devices[3]. We discuss the growth mechanisms of the ultrathin single crystal films. We conclude that the proposed growth methods can serve a promising platform for solution-processed ultrathin organic electronic devices.

This work was supported by Russian Science Foundation (grant 15-12-30031).

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P-12

In Situ Grazing Incidence X-ray Diffraction of Polymer-Fullerene Thin Films Under Thermal Treatment

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The polymer-fullenerene blends are important candidates for solar cell applications. We present in situ grazing incidence X-ray diffraction (GIXD) studies of polymer:fullerene thin films under thermal treatment with combined conductivity measurements.

We compare the characteristics of pure poly(3-hexylthiophene) (P3HT) with blends of P3HT with fullerene derivatives of either [6,6]-phenyl C61 butyric acid methyl ester (PCBM) or indene-C60 bisadduct (ICBA). Upon annealing the polymer exhibited a complex thermal behaviour: thermal compression in π-stacking direction whereas the stacking distance along the alkyl side chains expanded. In situ GIXD studies allow us to observe different temperature dependent features for the blends. In contrast to ICBA, the PBCM blends developed a pronounced and narrow diffraction peak at temperatures around 180 °C (Fig. 1). The measured electrical characteristics hint towards a strong contribution of the fullerenes to conductivity.

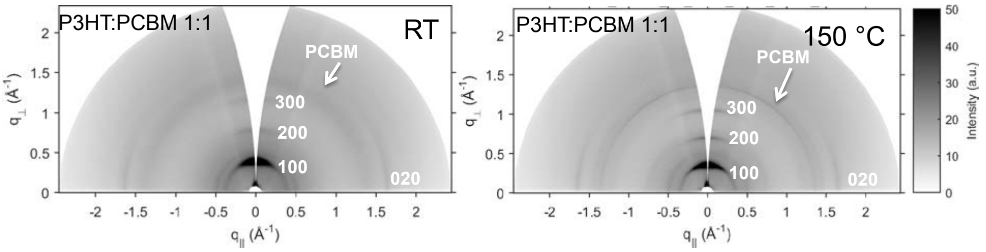

Fig. 1. 2D diffraction patterns of P3HT:PCBM blend at room temperature (left) and at 150 °C (right)

This work was supported by BMBF (project № 05K13PS4).

Analysis of $ASnI_3$ ($A = CH_3NH_3^+$ or Cs^+) and doped Cs_2SnI_6 perovskite-like structures

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Hybrid organic-inorganic halide perovskites having general formula AMX_3 where A is an organic or inorganic cation, M is ion of lead(II) or tin(II) and X is a halogen ion are the perspective light-absorbing compounds for solar cells. Since 2009 when the first perovskite-based solar cell was created the efficiency of this kind of devices has increased from 3.8% to 20%. The toxicity of the most standard light harvesting materials – lead halide perovskites – restricts their practical application. Replacement of lead in these compounds with divalent tin is a perspective way to make perovskite-based solar cells completely non-toxic without losses in efficiency and simplicity of its production. Another advantage of tin-based halide perovskites is lower band gap (for example, for tin(II)-methylammonium iodide it is about 1.20 eV compared to 1.5-1.6 eV for lead analog). It provides more complete light absorption of tin-based Grätzel cells. However, instability of divalent tin under ambient conditions causes rapid degradation of tin halide perovskites and restricts their application. The aim of the many researches connected with tin-based perovskites is the stabilization of these compounds.

In this work we studied the degradation processes of tin halide perovskites (tin(II)-cesium iodide and tin(II)-methylammonium iodide) obtained from the solutions in water or propanol-2 by heating in open air or long-term drying in inert atmosphere. These compounds were subjected to X-ray diffraction analysis right after crystallization and their degradation during one month of staying in open air. The same analysis was made with the tin(IV)-cesium iodide. Additionally, the absorption spectra of tin(II)-methylammonium iodide, tin(II)-cesium iodide and tin(IV)-cesium iodide samples right after synthesis and after few days of staying in open air are studied. Degradation of tin(II)-methylammonium iodide and tin(II)-cesium iodide after a one week of staying under high temperature (about 40 ^{o}C) or high moisture (above 60% compared to 20% in previous study) was analyzed in a same way.

The second aspect of research project was the synthesis and investigation of the properties of antimony(III)-doped tin(IV)-cesium iodide. Having appropriate electron conductivity and comparably low energy gap (about 1.3 eV) this compound is a perspective material for perovskite solar cells. One of the most important advantages of antimony(III)-doped tin(IV) cesium iodide is its stability under ambient conditions. At addition, this compound is completely non-toxic. The aim of our research was the investigation of phase composition of samples with different antimony content. In this work we produced the antimony(III)-doped tin(IV)-cesium iodide having general formula $Cs_2Sb_xSn_{1-x}I_{6-x}$ (where $0.05<x<0.30$) by the crystallization from tin(IV) iodide, cesium iodide and antimony(III) iodide solution in DMF using the spin-coating. These samples were studied by XRD and their band gaps were calculated from their absorption spectra.

P-14

Deposition of electroactive molecules in micro and nano gaps

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Deposition of organic molecules onto different surfaces faces with some complicated tasks, such as surface roughness and wettability, which highly affect the process. The main problem is how to deposit molecules directly into the gap between two electrodes. In this work we study the deposition of electroactive molecules into micro and nano gaps between gold and single-walled carbon nanotubes (SWCNTs) electrodes respectively.

SWCNTs were synthesized by Professor A. Nasibulin (Skoltech). They were deposited onto Si/SiO_2 substrate. Au/V 100/5 nm contacts were formed then by photolithography. Polyaniline (PANI) in emeraldine base form with an average molecular weight of 10000 and α,α'-dihexylquaterthiophene were used as electroactive molecules. PANI was dissolved in 1-methyl-2-pyrrolidone and dimethylacetamide, oligothiophenes were dissolved in non-polar solvents. We prepared solutions with different concentrations to find the optimal deposition conditions. Molecules were deposited onto a surface using drop coating technique from a solution. After that atomic-force microscopy was performed to determine the density and preferential places of molecules deposition (Figure 1a).

We found that oligothiophenes were not commonly deposited into micro and nano gaps and near metal contacts in crystal form like on clean SiO_2 substrate far from contacts, they form only poor conductive agglomerates. Also molecules prefer to deposite onto SWCNTs rather than onto dielectric substrate. For improving of the technique we used electrophoresis with AC and DC voltages with amplitude of 8 V and current limit of 100 nA (Figure 1b), which simplified the deposition of elecroactive molecules between contacts. But, for each material and size of molecules one needs to choose a specify frequency for the deposition. Varying the AC voltage frequency we found the range for PANI molecules deposition (Figure 1b). In order to reduce the size of the agglomerates, it is necessary to decrease the concentration and use ultrasonication before the deposition. We found that optimal concentration for oligothiophene and PANI molecules is 0.05 μg/ml. The maximum size of the agglomerates in this case is less than 10 nm.

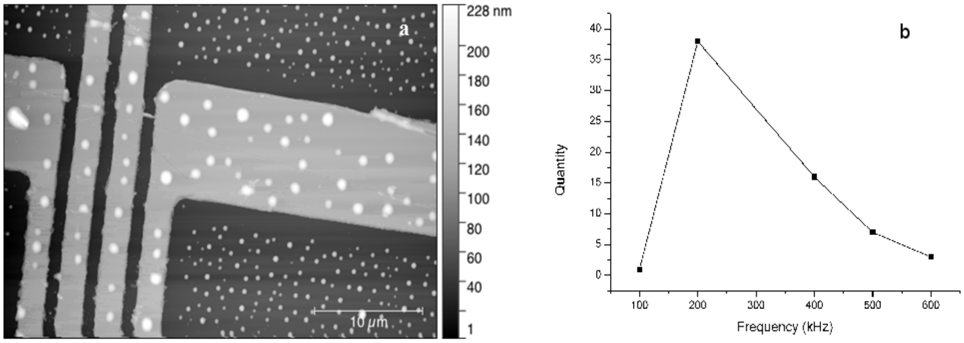

Figure 1. AFM images of the deposited oligothiophene molecules using drop-coating technique from a solution (a) and quantity of deposition molecules versus frequency dependent (b)

This work was supported by RSF (grant №14-19-01308).

P-15

Energy level tuning of PPDTBT polymers: towards high V_{oc}, low energy loss solar cells

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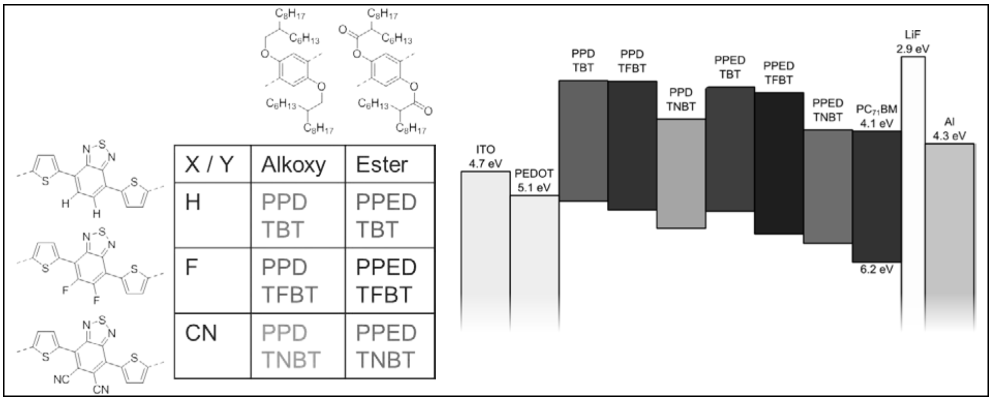
A precise control over the energy levels of conjugated polymers is important to allow for high voltage polymer solar cells, while retaining as much of the absorption range as possible. Dithienobenzothiadiazole containing polymers afford efficient medium and wide bandgap materials for polymer solar cells and provide a convenient handle for controlling the electronic properties. Together with alkoxy substituted phenylene, this type of polymer gave excellent power conversion efficiencies as was shown by Woo *et al.*[1].

Six polymers, containing differently substituted benzothiadizaole (**BT**) and phenylene (**P**) moieties, were synthesized in order to study the effect of substitution on the HOMO and LUMO levels of the conjugated polymers. Benzothiadiazole was substituted with hydrogen, fluorine or nitrile-groups, whereas the phenylene moiety was substituted with 2-hexyldecyl alkoxy side chains or their ester derivatives. The performance of the cells was correlated with the offsets of the HOMO and LUMO levels and morphology of the active layers as determined with transmission electron microscopy. Surprisingly, the highest power conversion efficiency (PCE) of 6.6% was not found for the polymer with the optimized energy levels, but for the polymer of which photoactive layer featured distinct phase separation and crystalline domains. As a result the fill factor and photocurrent improved, such that the PCE increased despite a relatively large photon energy loss (E_{loss} = 0.97 eV). In contrast, the polymer with the lowest E_{loss} (0.49 eV), gave a PCE of only 1.8%. Nevertheless, we consider this derivative as a potentially interesting material because it represents one of the lowest E_{loss} energies reported for organic solar cells, while still having an appreciable EQE of 17%. The EQE is, at least in part, limited by a sub-optimal morphology.



X / Y	Alkoxy	Ester
H	PPD TBT	PPED TBT
F	PPD TFBT	PPED TFBT
CN	PPD TNBT	PPED TNBT

Fig. 1. Different polymer substitution possibilities (left) and overall trend in energy levels of the resulting polymers (right).

The research has received funding from the European Research Council under the European Union's Seventh Framework Programme/ERC Grant Agreement No. 339031

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Solution cast nickel oxide thin films as efficient hole extraction layers in organic electronics

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In order to optimize power conversion efficiencies in hybrid multilayer solar cells, it is essential to improve charge carrier extraction after photo-excitation. To minimize recombination losses across device interfaces, carrier selective buffer layers of transition metal oxides have been used between absorber and metal contacts[1]. Thin films of nickel oxide have shown promising properties as hole contact material with high transparency, and a good matching ionization potential to most donor materials[2,3]. We employ a few nanometer thin nickel oxide layer by solution casting on ITO/FTO substrates at varying annealing temperatures between 275°C and 400°C to study the chemical composition and electronic properties upon processing conditions via XPS/UPS, IR-spectroscopy, scanning probe microscopy and four-point probe measurements. The nickel oxide films exhibit high reactivity and quite low p-type character after oxidation in ambient air and nitrogen atmosphere. While post-annealing in an oxygen deficient environment reduces excess interstitial oxygen, shifting the Fermi-level of the s-NiO_x film further into the bandgap, the increase in oxygen partial pressure under ambient atmosphere does not lead to a higher p-doping level. We assume that the partial pressure of oxygen in ambient leads already to a saturation of bulk interstitial oxygen. To reduce the surface reactivity and increase the work function, we passivate the surface with self-assembled monolayers of phosphonic acids from an ethanolic solution. We observe a conversion of $Ni(OH)_2$ species via the phosphonic acid binding group and a reduction of surface water. We build solar cells to correlate our analytical results with device performance.

This work is supported by the BMBF project INTERPHASE, FKZ13N13656.

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P-17

Low LMCT state lanthanide complexes as luminophores in phosphorescent and NIR-emitting OLEDs

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Due to the spin statistic rules the luminescence of organic luminophores is restricted by singlet excitons and cannot exceed 25% efficiency in OLEDs. To overcome the restriction the atoms of heavy metals (mostly Ir) are included into the molecules of luminophores. In this case, strong spin-orbital coupling makes it possible the emission from triplet level and, as a result, reach 100% luminescence efficiency. We assumed that for lanthanide complexes with low energy LMCT (Ligand to Metal Charge Transfer) state the ligand-metal orbital coupling, similar to that of Ir complexes having MLCT excited state, can take place what will lead to enhanced phosphorescence. In order to obtain low energy LMCT state lanthanide complexes thiolato type heterocyclic ligands 2(2´-mercaptophenyl)benzothiazole (SSN) and 2(2´-mercaptophenyl)benzoxazole (OSN) were chosen. Cyclic voltammetry revealed that these ligands in deprotonated form have reduced oxidation potentials as compared with its hydroxyl analogues and some β-diketones. Due to reducing abilities of the thioles H(OSN) and H(SSN) its reactions with amides of Eu^{3+}, results in reduction of europium to divalent state and formation of dithio derivative - bis[2-(2-benzothiazolyl)phenyl] disulfide. New binuclear $Ln_2(OSN)_6$ and mononuclear $Ln(SSN)_3$ complexes of Yb(III) and Gd(III) with thiophenolate ligands were synthesized by reaction of lanthanide amides $Ln[N(SiMe_3)_2]_3$ with respective thiophenols. Yb derivatives of these complexes have been structurally characterized (fig.1).

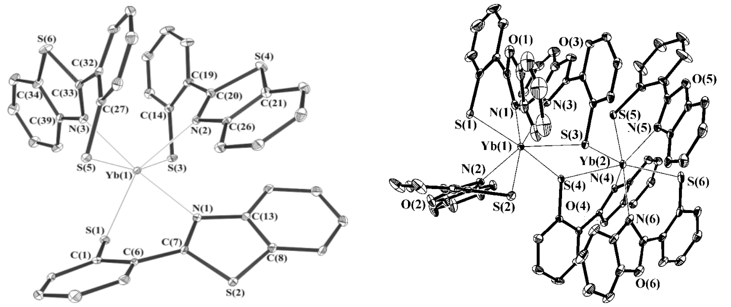

Fig. 1. Molecular structure of $Yb(SSN)_3$ (left) and $Yb_2(OSN)_6$ (right)

It was found that in solutions the compounds provides emission caused by fluorescence of keto and enol forms of the ligands. No energy transfer from organic part to Yb^{3+} ions has been detected in solutions of both Yb complexes, whereas in solids an intense metal-centered emission in near infrared region was observed. The solid Gd compounds exhibit room temperature phosphorescence caused by unusual efficient intersystem crossing which is facilitated by essential reducing properties of OSN and SSN ligands. To explain a sensitization process occurring in solid $Yb_2(OSN)_6$ and $Yb(SSN)_3$ a specific non-resonant energy transfer mechanism via LMCT state is proposed. The OLED device with carbazole: $Gd_2(OSN)_6$ (10%) emitting layer displayed triplet emission at 550 nm with brightness of 1350 cd/m^2 at 15V. The luminance intensity of OLED with neat $Yb_2(OSN)_6$ emission layer in NIR region reached 860 μW/cm^2.

This work was supported by RFBR (project № 15-33-20296 mol_a_ved).

P-18

Novel binuclear copper(I) complexes as perspective emitters for OLEDs.

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A series of new binuclear copper(I) complexes [Cu_2(N^N-$(CH_2)_4$-N^N)$(DPEphos)_2$]$(BF_4)_2$ (N^N = 2-(pyridin-2-yl)-1*H*-benzoimidazole, 2-(quinolin-2-yl)-1*H*-benzoimidazole, 4-(1*H*-benzoimidazol-2-yl)thiazole; DPEphos = bis(2-(diphenylphosphanyl)phenyl) ether) were synthesized (Fig. 1).

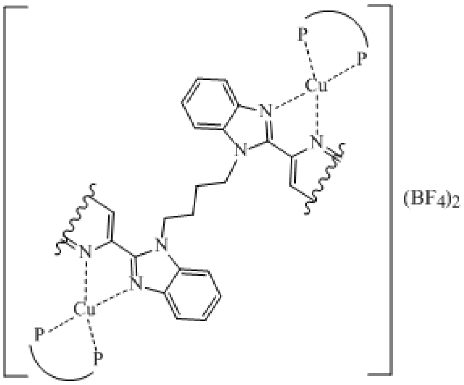

Fig. 1. Molecular structure of binuclear copper complexes.

The products are yellow solid substances that are stable in air and well soluble in THF, CH_2Cl_2, and $CHCl_3$. All compounds were characterized by elemental analysis, TGA, IR, UV-vis, and NMR spectroscopies.

To study the electroluminescent properties of the copper complexes, model OLED devices ITO/PVK:Cu-complex/BATH/Alq_3/Yb were fabricated. Various dopant concentrations from 5 to 20 wt% were used. The layer of indium oxide doped with tin oxide (ITO) served as the anode. The role of the emission layer was played by binuclear copper complexes. 4,7-Diphenyl-1,10-phenanthroline (BATH) and aluminium tris(8-oxyquinolinate) (Alq_3) were used as the hole-blocking and electron-transporting layers, respectively. The layer of metallic ytterbium served as the cathode. The value of brightness >1100 cd/m^2 was achieved for dopant concentration of 5 wt%. OLEDs generated luminescence of orange, yellow and green colours depending on the nature of N^N-ligands.

This work was supported by RFBR (projects № 16-33-00090, №15-03-02467).

P-19

Synthesis and properties of dendritic organosilicon luminophores with various central acceptor groups

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Organic luminophores are functional materials for a variety of optoelectronic devices, which are used in photonics, organic electronics, medical diagnostics and many other fields. In this work, we synthesized and investigated two new dendritic organosilicon luminophores, (PTPTP)Si_6(2T-Hex)$_{12}$ and (DPAnt)Si_6(2T-Hex)$_{12}$ (Fig. 1), which are one of the types of the so called “nanostructured organosilicon luminophores” (NOLs)[1,2], NOLs are a kind of highly efficient dendritic molecular antennas[3], consisting of donor and acceptor fragments covalently linked through a silicon atom with highly efficient intramolecular energy transfer between them by Förster mechanism.

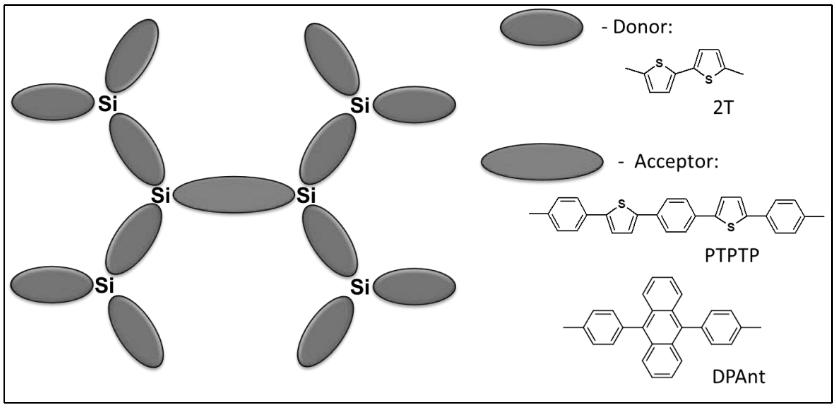

Fig. 1. Schematic representation of (PTPTP)Si_6(2T-Hex)$_{12}$ and (DPAnt)Si_6(2T-Hex)$_{12}$ synthesized and investigated.

These molecules consist of 12 donors and one acceptor luminophore located in the center. They have a high efficiency of energy transfer from the donor to the acceptor, and show a luminescence quantum yield 84% at excitation wave length is 336 nm for (PTPTP)Si_6(2T-Hex)$_{12}$ and 87% at 334 nm for (DPAnt)Si_6(2T-Hex)$_{12}$. The goal of this work was to compare the optical properties of the molecules synthesized to each other as well as with their smaller analogues (PTPTP)Si_2(2T-Hex)$_4$ and (DPAnt)Si_2(2T-Hex)$_4$ synthesized earlier.

This work was supported by Russian Foundation for Basic Research (grant 16-03-01118).

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P-20

Obtaining of the thin layers of $CH_3NH_3PbI_3$ and ZnO for application in solar power engineering

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Photovoltaic devices based on perovskite compounds is the promising mainstream in solar power engineering because of their cheapness compared with other types of solar cells. Organic-inorganic perovskites were proposed as light harvesting materials for photovoltaic cell since 2009 the efficiency of the first perovskite solar cell was 3.8%. During the next seven years the efficiency of perovskite-based cells was increased more than five times and achieved 22.1 % in 2016.

This work was focused on synthesis and physicochemical analysis of composite films $CH_3NH_3PbI_3$/ZnO. Zinc oxide is the possible analogue of titanium dioxide which demonstrates higher carrier motilities both for electron and holes. Thin films of zinc dioxide were obtained by spin-coating method using different colloidal solutions of ZnO nanoparticles (10-20 ± 3 nm diameter) in alcohols and mixed solvents. Characteristic diameter of particles strongly depends on temperature of the primary synthesis process. Dozens of nanometers thick ZnO films were produced.

Micromorphology, phase composition and resistance of the films were controlled by electron microscopy, XRD, diffuse reflectance spectroscopy, electrochemical impedance spectroscopy methods, correspondingly. It was established that the problem of ZnO thin film made from ZnO nanoparticles is incomplete coverage of conducting ITO surface. As a solution, a portion of terpineol was added to the planting mixture to make the resulting ZnO film thinner and more regular.

The deposition method to form even coatings of a standard organic-inorganic perovskite sensitizer $CH_3NH_3PbI_3$ was optimized for substrates with fine ZnO films coatings. That was observed also that $CH_3NH_3PbI_3$/ZnO films deposited by one-step crystallization method from different solvents (i-C_3H_7OH, n-C_4H_9OH, DMSO, DMF) decomposed with unequal rates when exposed in moist atmosphere or sintered at 100-150°C. Such an effect originated from micromorphology peculiarities of the perovskite phase and, likely, oxygen conductivity of zinc oxide.

P-21

Synthesis of novel pyrimidine derivatives of D-[π]-D type containing heterocycles and TTF moieties

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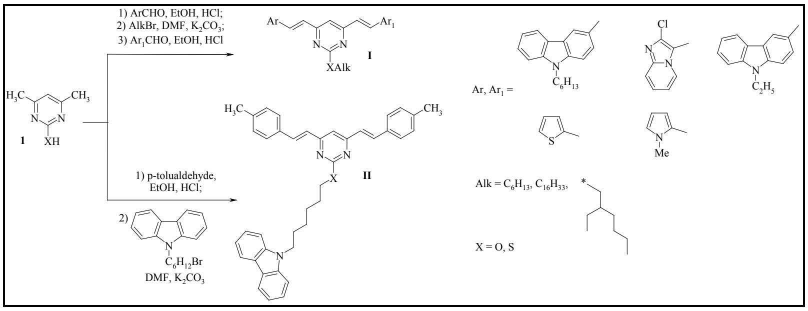
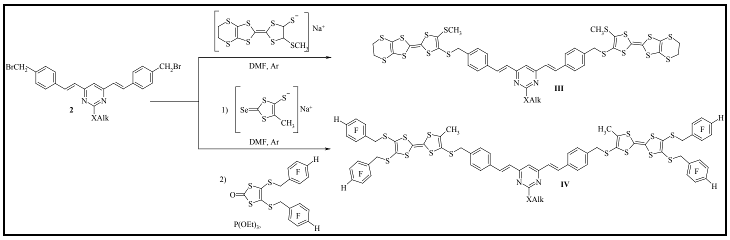
It is known that, chromophore structures of D-[π]-A-[π]-D type, where A is a pyrimidine core are investigated with a point of view of their potential application in organic devices such as OLEDs, thin film OFETs, solar cells and chemosensors. Recently we have synthesized a set of new conjugated compounds incorporating a 2,4,6-trisubstituted pyrimidine core[1,2]; their optical and electrochemical properties were studied. As the obtained compound have revealed good film forming properties we have prepared some thin films and studied their morphology with help of AFM and STM. The examples of the applied synthetic procedures are shown in Schemes. The compounds of **I** and **II** groups have demonstrate strongly pronounced solvatochromic properties and a hole type of conductivity.



4,6-Distyrylphenylsubstituted pyrimidines **III** and **IV** containing terminal TTF fragments have also demonstrated good film-forming properties. As the compound **IV** includes 16 fluorine atoms it is expected to exhibit conductivity of n-type [3].



This work was supported by The Ministry of the Education and Science of the Russian Federation (012011461916) and by RFBR (project 14-03-00341a, 14-03-96003p_ural_a). The instrumental investigations were fulfilled with equipment obtained by National Research University program.

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P-22

Solid photoluminescence standard based on an organosilicon luminophore

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Absolute measurements of photoluminescence (PL) quantum yield (QY) can be done by using PL standards, which should satisfy the following requirements: simple preparation of samples and their reproducible optical properties, high PL QY and its stability during the measurement and storage (absence of degradation), weak PL reabsorption, and wide PL spectrum.

Dilute liquid solutions of various dyes are widely used as PL standards for absolute PL QY measurements in solution[1]. Nevertheless, for various solid samples, whose PL QY needs measurements with an integrating sphere[2], liquid standards are inconvenient to verify the measurement procedure, and solid ones are preferable; however, they are not commonly used. In this work, we show that solid solution of a organosilicon luminophore 4,7-bis(4'-(trimethylsilyl)-[1,1'-biphenyl]-4-yl)benzo[c][1,2,5]thiadiazole (Fig. 1) is promising as a solid PL standard. Solid solution of the luminophore was prepared in a paraloid film, whose absorption and PL spectra are shown in Fig. 1. The film shows strong PL in nearly the whole visible spectral range with high Stokes shift, which provides low PL reabsorption. The absolute PL QY measured by using a calibrated integrating sphere (Newport, 3.3 inch, Spectralon coated) was close to 100 %. The PL spectrum and QY were measured repeatedly many times and did not show any signatures of aging. We conclude that the organosilicon luminophore dispersed in a solid matrix can be applied as a robust solid PL standard in various luminescent studies especially of solid samples, for example, organic crystals. The solid PL standard is very useful for the integrating sphere method as it allows avoiding its absolute calibration.

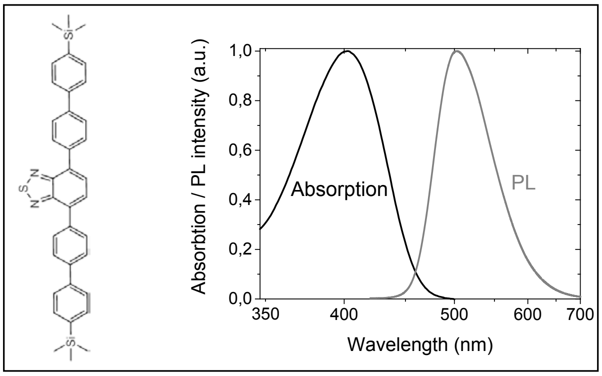

Fig 1. Chemical structure of the luminophore; absorption and PL spectra of the solid solution. The PL spectrum was recorded with an integrating sphere at 405–nm excitation

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P-23

Theoretical study of annulation effect in O- and S-containing five-ring heterocyclic rod-like molecules on their optical and electronic properties

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Thiophene- and furan-containing conjugated molecules are of great interest in organic optoelectronics because of their potential applicability in semiconducting and various light-emitting devices.[1,2] Prediction of optical and electronical properties of the molecules allows to better understand the phenomenon and to preselect perspective materials in silico before their synthesis in laboratory. One of the most important parameters affecting the charge transport is the intramolecular reorganization energy, defined as energy dissipation due to geometry changes between charged and neutral states during the charge transport, which is strongly related to the charge mobility according to Marcus theory.[3] In this work we computationally investigated the influence of annulation effect in O- and S-containing five-ring heterocyclic rod-like molecules (Fig. 1) on reorganization energy, frontier orbitals delocalization and nature of excitation transitions.

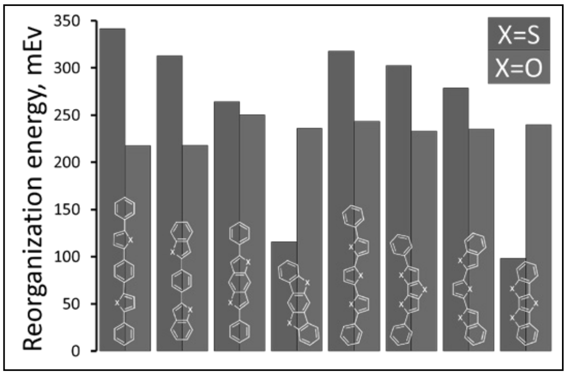

Fig. 1. Structural formulae of studied compounds and reorganization energy for hole transfer.

By using DFT B3LYP(+D3BJ)/Def2TZVP level of theory, it was shown that the annulation in S-containing molecules leads to a decreasing of intramolecular reorganization energy, whereas for O-containing analogs the reorganization energy does not significantly change probably due to their higher rigidity. We also predicted the absorption spectra at TD-DFT (CAM-B3LYP/6-31+G*) level, and it was shown that absorption maxima are hypsochromically shifted upon annulation due to more efficient conjugation.

We therefore concluded that, according to our study, annulated thiophene-containing condensed conjugated molecules are more perspective as semiconducting materials due to lower intramolecular reorganization energy, whereas annulation in furan-containing molecules has low impact on the charge mobility.

This work was supported by RFBR (project 16-33-60011).

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P-24

Novel conjugated organosilicon oligomers based on 2,1,3-benzothiadiazole

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Organic electronics is a rapidly developing field of science and technology[1]. It relies upon printing technology for creation of different electronic and optoelectronic devices with unique properties, such as flexibility, energy efficiency and low weight[2]. Conjugated oligomers are one of the widely used semicondicing materials in organic electronics, since they can be obtained as highly pure individual compounds, which are necessary for creation of effective devices. Among the oligomers we selected molecules containing 2,1,3-benzothiadiazole (BTZ) fragments, since they possess high thermal stability, large absorption coefficient and large Stokes shift[3]. Such properties of BTZ-based oligomers make it possible to apply them as excellent luminescent materials in various optoelectronic applications.

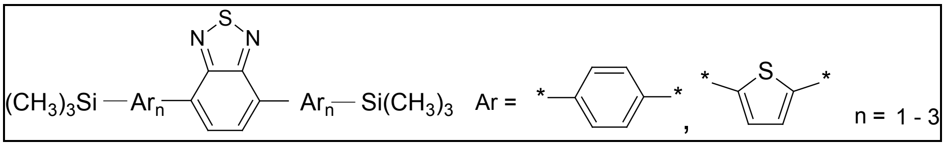

Fig.1. Chenical structure of the conjugated organosiliconoligomers based on BTZ.

The aim of this work was to synthesize a series of new push-pull conjugated oligomers, based on BTZ acceptor and various combinations of 2,5-thiophene and 1,4-phenylene donor units with trimethylsilyl and groups, as well as to study their optical and thermal properties (Fig.1). We have found that increasing the conjugation length leads to a significant red shift of both the absorption and luminescence spectra. The photoluminescence quantum yield (PLQY) of the oligomers containing only 1,4-phenyl donor fragments are higher than those of the oligomers containing 2,5-thiophene fragments and varies in the range of 20-95%. Increasing the conjugation lengh leads to a significant derease of solubility. Chemical nature of the donor fragment attached to the central BTZ group has the greatest influence on melting point of the oligomers. These new compounds due to their good optical properties are promising material for various organic optoelectronic applications.

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Reduced charge carrier trapping by controlled polymer blend phase dynamics

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In 1962 Mark and Helfrich[1] derived an expression showing the dependence of the current density in an organic crystal on the charge transport and trap site densities in the material. Their theory predicts that if the trap energy is distributed rather than discrete, spatial separation of sites leads to an increase in current density by elimination of its trap-limited nature. We recently validated Helfrich's theory for disordered (polymeric) semiconductor thin films. We demonstrated a pronounced increase in the otherwise strongly trap-limited electron current in poly(p-phenylenevinylenes)[2], by blending with poly(vinylcarbazole) (PVK) as insulating, and therefore electrically inactive, host. Interestingly, the effect was observed despite spinodal decomposition of the blend solution during film casting. To elucidate the link between phase behavior and the increase in electron current, we proceed with blending PPV with different insulators, most prominently polystyrene (PS)[3]. By varying the molecular weight of the insulator we tune the miscibility with the semiconductor and control the morphology of the dry film. Comparing the phase diagram, morphology (Figure 1) and current density obtained for the PPV:PS films with the corresponding data obtained for the PPV:PVK blend, we conclude that neither the question whether demixing occurs or not, nor the electronic properties of the individual blend constituents, but rather the composition of the coexisting phases determines the increase in electron current density.

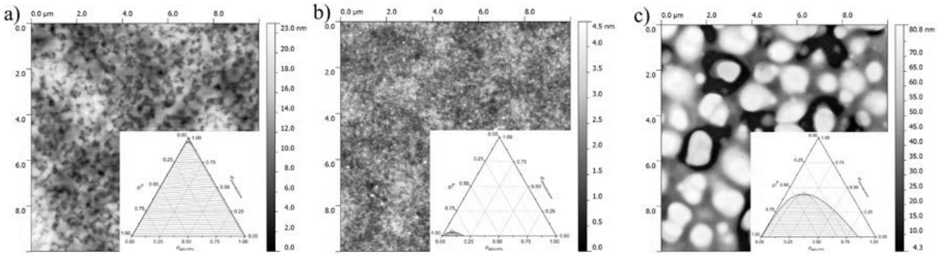

Figure 1: AFM surface topography images of 1:3 blend thin films of a) MEH-PPV:PS35, b) MEH-PPV:PS1, c) MEH-PPV:PVK. The insets show the corresponding calculated ternary phase diagrams including the solvent. An increase in electron current density is observed only for b) and c) owing to (coexisting) phases with mixed composition, in agreement with the phase diagrams.

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P-26

Polyaniline/polyethylene oxide memristors with planar thin-film or 3D fibrous architecture

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Memristors are non-volatile electronic elements with a resistance determined by the leaked charge history. Memristors could be prepared by planar thin-film technology[1] or based on fibrous materials[2]. Functionality of such memristors is based on electrochemical control of oxidation state of polyaniline film. Thin-film organic memristor based on polyaniline and silver chloride electrode separated by polyethylene oxide doped with lithium ions. Performance of electrochemical reactions is usually limited by ion diffusion speed through the interface. The memristors with 3D fibrous architecture have high surface and they are promising to create both a single devices and stochastic neural networks.

In this work the planar thin-film organic memristor was prepared by sequential deposition onto the substrate with titanium electrodes 1) polyaniline film, 2) a layer of electrolyte matrix doped with lithium ions and 3) silver chloride electrode. The polyaniline Langmuir films was transferred onto the substrate by Langmuir-Schaefer method. The polyaniline layer became conducting after doping deposited film in HCl solution or if acid solutions were used as the subphases in a Langmuir trough. The molecular structure of polyaniline Langmuir films onto pure water or acid solutions have been identified by X-ray diffraction in grazing incidence geometry («Langmuir», Kurchatov Institute Synchrotron Radiation Source).

There were different ways to prepare a memristor based on fibrous material. Nonwoven polymeric material may be impregnated with a solution of polyaniline or spun directly from polyaniline-containing mixture. The nonwoven materials for memristors with 3D microfiber architecture were prepared from the solutions of various polymers or their mixtures with polyaniline by electrospinning method. The resistance of polyaniline thin films or hybrid polyaniline-contained nonwoven materials and the current-voltage characteristics of the memristors based on such materials were measured.

This work was partially supported by grant of the President of the Russian Federation for the state support of young Russian scientists (MK-5779.2015.3) and RFBR (projects № 16-33-80147 and № 15-29-01324).

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P-27

Photoluminescence Anisotropy in Organic Semiconducting Single Crystals

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Single crystals of thiophene-phenylene co-oligomers (TPCO) have demonstrated high potential for organic optoelectronics as they combine high charge carriers mobility and bright luminescence[1,2]. Various remarkable luminescence properties such as the spectrally-narrowed emissions[3], self-wave-guide effect[4], lasing[4], and anisotropy of emission[3] have been observed for the different TPCO crystal structures. Photoluminescence (PL) anisotropy reveals the average angular displacement between the absorption dipole moment and the emission one exposing the details of the electronic transitions within the crystalline structure. Thus, PL anisotropy studies can provide additional insights into high luminescence yield in TPCO crystals that has not been fully understood yet.

In this contribution, we analyze anisotropy and kinetics of PL in single crystals of a novel TPCO (Fig.1a, top) 1,4-bis{5-[4-(trimethylsilyl)phenyl]thiophen-2-yl}benzene (AC5-TMS). Crystals were grown from solution and from the vapor phase. X-ray data show that the molecules are nearly flat-lying in the plane of the crystal plate (Fig.1a, bottom). PL spectra of the crystal are clearly different for X- and Y-polarized excitation (parallel and orthogonal to molecules backbones; Fig.1b), with the 450-nm band absent for the Y-polarized excitation. Surprisingly, the highest PL was observed for excitation polarization nearly orthogonal to the AC5-TMS backbone. However, PL is mainly polarized along the backbone regardless of the excitation polarization (Fig.1c). With the increase of the excitation wavelength from 400 to 445 nm, each PL spectral band decays noticeably slower (Fig. 1d). We will discuss the experimental data in the framework of the Davydov splitting model for AC5-TMS crystal packing.

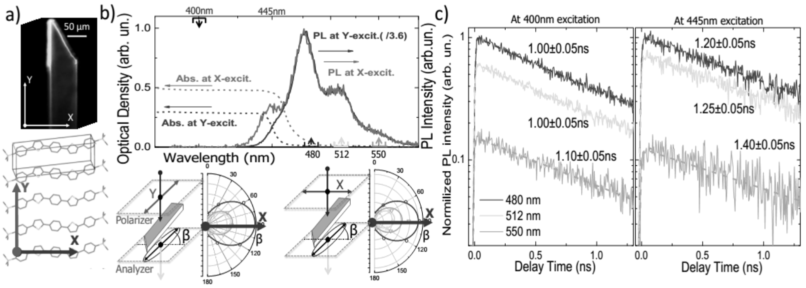

Fig.1 **(a)** Image of the AC5-TMS single crystal (top) and molecular packing (bottom); **(b)** Absorption and isotropic PL spectra for X- (cyan dash and solid, respectively) and Y-polarized excitation at 400 nm (red dash and solid); **(c)** Experiment geometries and PL anisotropies of spectral bands (480nm is blue; 512nm is green; 550nm is orange) for Y- (left) and X-polarized excitation at 400nm (right); **(d)** Spectral-resolved PL kinetics for 400nm (left) and 445nm excitation (right). The transients were averaged over the spectral ranges shown in (b) The dash lines are monoexponential fits convoluted with an apparatus response of 20 ps.

This work was partially supported by Russian Science Foundation (project № 15-12-30031).

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P-28

Highly soluble and thermally stable star-shaped oligomer for organic solar cells

A.L. Mannanov[1*], *V.A. Trukhanov*[1], *A.N. Solodukhin*[2], *Yu.N. Luponosov*[2], *S.A. Ponomarenko*[2], *D.Yu. Paraschuk*[1]

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The efficiency and stability of organic solar cells is still lower than those of inorganic solar cells. The performance of small-molecule organic solar cells (OSC) has been dramatically increased for the recent years. Oligothiophenes are among the most promising materials for small-molecule organic solar cells, e.g., OSC based on star-shaped oligothiophenes (SSO) with a triphenylamine donor core and dicyanovinyl acceptor terminal groups show the efficiency up to 5.4% [1].

In this work, we study OSC based on novel SSO N(Ph-2T-DCN-Ph)$_3$ and compare it with well-studied SSO N(Ph-2T-DCN-Et)$_3$. This alkyl-free star-shaped oligomer with electron-withdrawing phenyldicyanovinyl groups possesses a unique combination of extremely high solubility (up to 325 g/L in ODCB) and thermal stability (up to 490 ºC) with promising photovoltaic performance. The photovoltaic properties of N(Ph-2T-DCV-Ph)$_3$ were investigated in solution-processed bulk heterojunction OSC in the conventional structure glass/ITO/PEDOT:PSS/N(Ph-2T-DCV-Ph)$_3$:PC$_{70}$BM/Ca/Al. These OSC demonstrated an efficiency of 4.4%. For comparison, OSC based on N(Ph-2T-DCN-Et)$_3$ showed an efficiency of 4.5%. To optimize the morphology of the active layer, we used various fabrication protocols including thermal and solvent-vapor annealing, high-boiling solvent additives and others. We have found that a combination of hot solution spin-coated on a hot substrate and solvent-vapor annealing results in the best performance N(Ph-2T-DCN-Ph)$_3$ OSC.

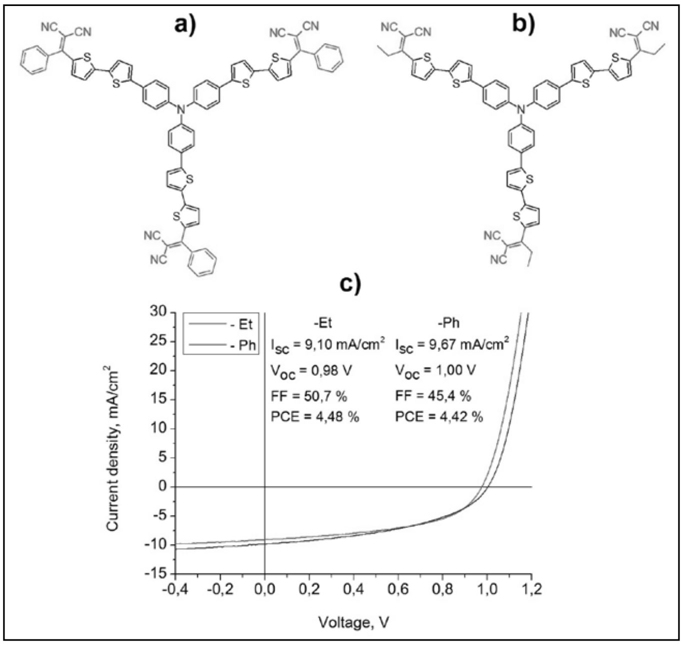

Fig. 1. (a), (b) Structural formulas of SSO N(Ph-2T-DCN-Ph)$_3$ and N(Ph-2T-DCN-Et)$_3$;
(c) I/V curve for N(Ph-2T-DCN-Ph)$_3$/PC$_{70}$BM and N(Ph-2T-DCN-Et)$_3$/PC$_{70}$BM solar cells.

This work was supported by RSF (project № 14-13-01380).

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Surface-enhanced Raman spectroscopy of semiconducting monolayers

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Organic semiconducting monolayers have high potential for ultrathin electronics[1]. The best monolayer electronic devices are based on crystalline monolayers. However, the local monolayer order has practically not been studied. To probe the monolayer domain structure with the spatial resolution less than 1 um, Raman spectroscopy can serve as a useful tool.

In this work, we report Raman study of semiconducting monolayers D2-Und-4T-Hex and O(Si-Und-PTTP-TMS)$_2$ (Fig 1. a, b) prepared by Langmuir technique. As the monolayers give a very weak Raman signal, to amplify it, we apply surface-enhanced Raman spectroscopy (SERS). To maximize the SERS signal-to-noise ratio(s/n), a Si substrate with gradual varying gold thickness (10–70nm) was prepared and then a monolayer film was deposited. The dependence of SERS s/n on the gold thickness shows the maximum at 20 nm. (Fig 1, c) We succeeded in obtaining Raman map for D2-Und-4T-Hex (Fig 1. d, e) and O(Si-Und-PTTP-TMS)$_2$. Using optical and atomic force microscopies, we found that D2-Und-4T-Hex films have a domain structure, where O(Si-Und-PTTP-TMS)$_2$ films do not. We discuss how the Raman maps are associated with structural features of the monolayers.

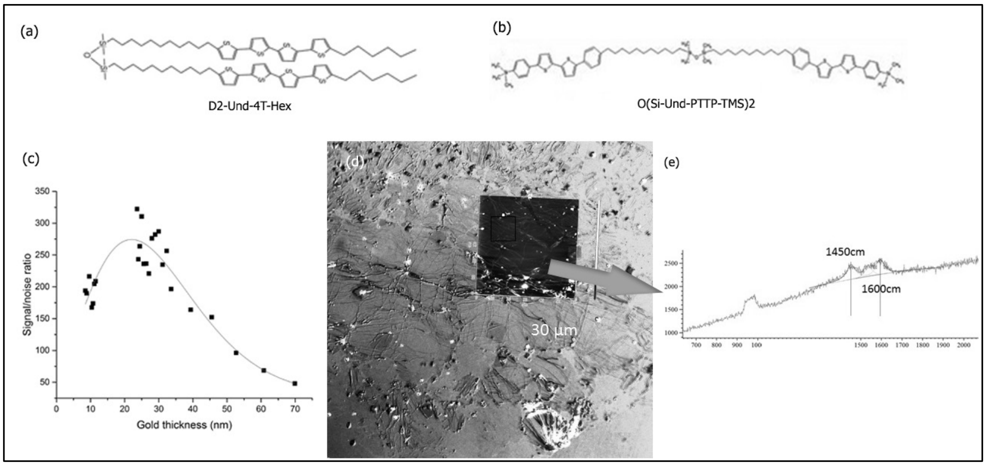

Fig.1. Chemical formula of (a) D2-Und-4T-Hex and (b) O(Si-Und-PTTP-TMS)$_2$. (c) SERS signal-to-noise for O(Si-Und-PTTP-TMS)$_2$ monolayer. (d) Microscope image of the monolayer (C-DIC) and (e) Raman map from the selected area of D2-Und-4T-Hex. Red laser (633nm) with a power of 20mW was used for Raman excitation. Langmuir–Blodgett films were prepared using toluene solution with the concentration of substance of 0.33 g/l.

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Charge-Transfer – Solvent Interaction Predefines Doping Efficiency in p-Doped P3HT-Films

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Efficient electrical doping of organic semiconductors is a necessary prerequisite for the fabrication of high performance organic electronic devices. Numerous recent publications emphasize the need for further investigations, especially on polymer systems. In this work, we study p-type doping of poly(3-hexylthiophene) (P3HT) with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F_4TCNQ). Using electron diffraction, performed in a transmission electron microscope, we find strong dopant-induced π-π-stacking for films spin coated from the low boiling-point solvent chloroform, but not from the high boiling-point solvent chlorobenzene. This image is confirmed and expanded by the analysis of vibrational features and polaron absorptions using Infrared and UV-Vis absorption spectroscopy. These differences result in a higher conductivity of films from chloroform. We use optical spectroscopy on the corresponding blend solutions to shed light on the origin of this effect and show that structural order and electronic properties in doped films are predefined by the interaction of the solvent with charge-transfer complexes already in solution. Our study emphasizes the importance of solvent parameters exceeding the bare solubility of pure dopant and host material for the preparation of highly conductive doped films.[1]

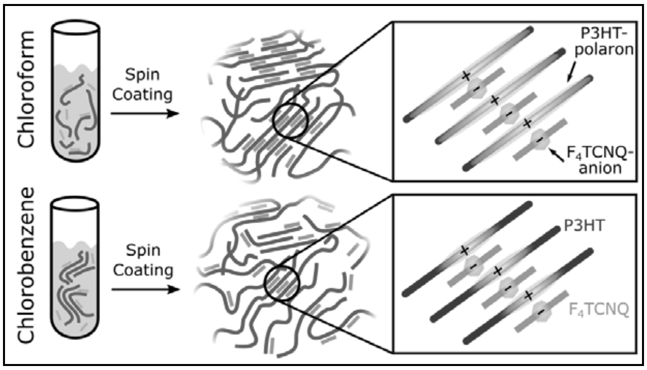

Fig. 1. Schematic drawing and summary of the observed effects from the solution state to dried thin films of P3HT:F_4TCNQ.

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[1] Müller et al., *Chemistry of Materials*, Article ASAP, DOI: 10.1021/acs.chemmater.6b01629

P-31

Efficient modeling of conjugated polymers for electronics and energy storage

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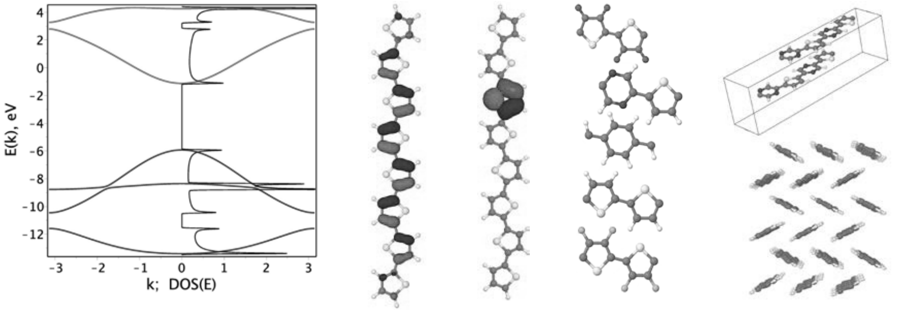

(a) (b) (c) (d) (e)

Fig. 1. (a) Structure of π-bands and the corresponding electronic density of states for polythiophene; (b) The HOMO wavefunction; (c) Three types of localized molecular orbitals entering the tight-binding model of hole bands; (d) Examples of considered building blocks; (e) Two types of intermolecular packing studied: π-stack and herringbone structures.

Ongoing materials research for organic electronics faces a problem of an enormously large exploration space, which to some extent can be solved by multiscale modeling. In particular, combining computational methods at several scales makes it possible to extract such key mesoscale properties of organic polymers as charge-carrier mobility, including the account for polaronic effects and/or disorder,[1] and to relate them to morphology of bulk materials.

We develop efficient methods for modelling of various conjugated polymer systems, from single chains to π-stacks, polymer bundles, and crystals. The developed methods are then applied to studies of organic cathode materials,[2] solar cells, and field-effect transistors.[3] On the materials side, we examine morphology and electronic properties of polymers shown in Fig. 1, as well as other systems of interest.

To model structural properties, we use classical molecular dynamics with OPLS-type force field. The missing parameters are obtained from DFT calculations. The force field is tested on separate chains and bundles;[4] the results are then compared to MM3 and DFT calculations. The adjusted force field is used to compute morphological structures of molecular crystals and polymer bundles. Electronic properties of thus simulated structures are computed using a localized molecular orbital approach, which allows to reduce the complexity of quantum chemical calculations to a tight-binding level while preserving a DFT-level accuracy.

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Red light-emitting polynorbornenes with cyclometaled iridium(III) complexes in side chains

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New polymerizable cyclometaled iridium(III) complexes (NBEpz)Ir(Btp)$_2$ (**I**) and (NBEpz)Ir(Piq)$_2$ (**II**) (NBEpzH is 1-phenyl-3-methyl-4-(5-bicyclo[2.2.1]hept-5-en-2-yl)-5-pyrazolone, BtpH is 2-(benzo[*b*]thiophen-2-yl)pyridine), Piq is 1-phenylisoquinoline) were synthesized. Norbornene based iridium-containing monomers **I** and **II** were copolymerized with carbazole-containing comonomer via Ring-Opening Metathesis Polymerization. The formed polymeric products (Fig. 1) revealed an intense photoluminescence (PL) and electroluminescence (EL) of red color.

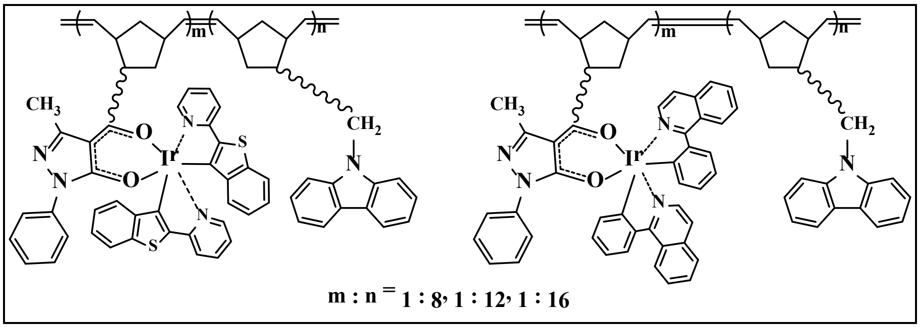

Fig. 1. The synthesized iridium-containing copolymers.

All polymeric products were characterized by elemental analysis, IR-, MNR-spectroscopy, GPC, TGA. Their photophysical properties were investigated. PL and EL spectra of the copolymers contained emission bands attributed to pendant iridium complexes and no emission from carbazole groups was observed. Model OLED devices based on iridium polymeric emitters - ITO/Ir-polymer/BATH/Alq$_3$/Yb showed maximum brightness up to 1100 cd/m^2, maximum current efficiency – 17.9 cd/A, maximum power efficiency – 9.1 lm/w. The reached values of current efficiency and power efficiency are the highest performance characteristics among the known electroluminescent iridium-containing red-emitting polymers.

T*his work was supported by the Russian Foundation for Basic Research (Projects No. 16-33-00234-mol_a, No. 15-43-02178-r_povolzh'e_a).*

P-33

Solution-grown large-area ultrathin films of α,α'-dihexylquinquethiophene for organic field-effect transistors

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Charge transport in organic field-effect transistors (OFETs) occurs in a few molecular layers adjacent to the gate dielectric. This stimulates researchers to develop monolayer field-effect devices with a thickness of one/few molecular layers. The most successful monolayer OFETs were realized on oligothiophenes using molecular self-assembly in solution[1] or Langmuir technique[2]. For these techniques, one needs semiconducting molecules with special functional end groups that calls for complicated synthetic chemistry.

In this work, we present a simple and robust solution-based technique for fabrication of large-area ultrathin films of α,α'-dihexylquinquethiophene (DH-5T) and demonstrate their functionality as active layers of organic field-effect transistors (fig. 1 a). DH-5T films were fabricated by spin-coating from solution on a SiO_2/Si wafer with subsequent annealing in the saturated solvent atmosphere. Tuning the film processing conditions such as concentration, solvent, spinning speed and time, annealing temperature, we managed to fabricate smooth monolayer-thin large-area (~10 mm^2) films (fig. 1 b, c) without optically visible defects. Bottom-gate OFETs with printed PEDOT:PSS top-contacts showed excellent performance demonstrating the hole mobility ~0.02 cm^2/Vs, which is one of the highest among monolayer OFETs[i] (fig. 1 d). We discuss the growth mechanism[3] of the DH-5T films and their structure. We conclude that the presented technique for fabrication of large-area ultrathin semiconducting films is promising for organic electronics printing technologies.

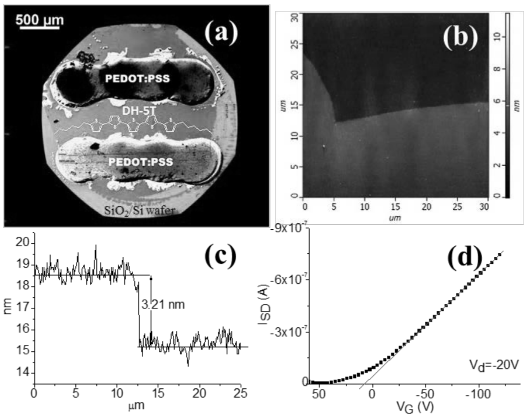

Fig. 1 Optical image of the fabricated device **(a)**; AFM image of the film surface **(b)** and the film profile **(c)**; OFET transfer characteristics **(d)**.

This work was supported by RFBR (project № 16-32-50045).

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P-34

Synthesis and properties of novel organosilicon derivative of [1]benzothieno[3,2-b][1]-benzothiophene

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Currently, one of the promising directions of materials chemistry is design, synthesis and investigation of organic semiconducting materials, which can be used in organic electronics devices, such as organic light-emitting diodes (OLEDs), organic photovoltaics (OPVs) and organic field-effect transistors (OFETs)[1], including self-assembled monolayer field-effect transistors (SAMFETs)[2]. Compounds based on [1]benzothieno[3,2-b][1]-benzothiophene (BTBT) are promising materials for such devices due to their record high field-effect mobilities[3]. Recently we elaborated a novel fast, easily processible and highly reproducible approach to SAMFETs fabrication by Langmuir techniques[4]. As semiconducting materials we have used siloxane dimers with undecylic (C11) spacers between the conjugated thiophene-based units and central tetramethyldisiloxane fragment of the molecule[5].

In order to study the influence of the aliphatic spacer length on SAMFET performance, we synthesized a novel siloxane dimer with shorter (C7) aliphatic spacers connecting conjugated BTBT fragments with the disiloxane O(Si-Hept-BTBT-Hex)$_2$ (Fig.1). The synthesis was carried out using Kumada, direct C-H arylation and hydrosilylation reactions. The structure and purity of all intermediate and final compounds were confirmed by HPLC, ^{1}H-, ^{13}C-, and ^{29}Si-NMR spectroscopy, as well as elemental analysis.

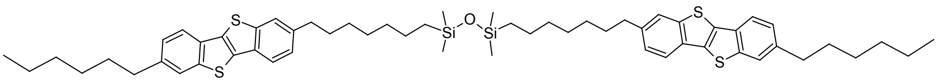

Fig. 1. Structural formula of O(Si-Hept-BTBT-Hex)$_2$ synthesized and investigated.

Semiconducting properties of the new material synthesized have been investigated in the monolayer OFETs fabricated by Langmuir-Blodgett (LB) and Langmuir-Schaeffer (LS) techniques in the bottom-contact bottom-gate geometry. The dimer demonstrate Langmuir isotherms and Brewster micrographs typical for crystalline films. Morphology of LB and LS semiconducting monolayers corresponds to fully covered highly-ordered monolayers with vertical orientation of BTBT fragments, small amount of holes and separate regions of bilayer. The saturated hole mobilities were measured as 2×10^{-2} cm^2/Vs with the threshold voltage near 0V and on/off ratio about 10^3 (Fig.2). Thus, LB SAMFET based on this novel siloxane dimer of BTBT showed excellent semiconducting properties comparable to those obtained by solution-processed self-assembly.

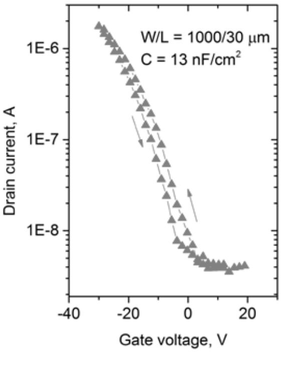

Fig.2 Transfer curve of LS monolayer OFET.

This work was supported by RFBR (project № 16-29-05321).

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P-35

Sensitization of NIR emission of Nd3+ by Zn-containing Schiff base complex

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Near infrared (NIR) luminescent lanthanide complexes attracts great attention of researchers working in the fields of optoelectronics and biomedicine, since these materials can be exploited as emissive materials for OLEDs, dopants for polymer optical fibers communicating signals in the transmission windows and phosphorescent probes for bioimaging. Efficiency of Ln^{3+} ion metal-centered photoluminescence (PL) as well as its lifetime strongly depend on geometry of metal coordination polyhedra and energetic characteristics of organic ligands which harvest energy of the incident light and transfer it to rare earth center. It was shown that f-f emission can be enhanced by means of energy transfer from zinc containing chromophore groups coordinated to Ln^{3+}.[1,2] In order to investigate sensitization effect of Zn-containing fragments we synthesized the complexes Zn(L) (**1**), $NdCl_3$•(H_2L) (**2**) and $NdCl_3$•(Zn(L)) (**3**) (Fig. 1a), where L is salen type Schiff base ligand. The complex **1** has shown intense yellow emission (λ_{max} = 575 nm) upon 410 nm excitation (Fig. 1b) while H_2L does not reveal any luminescence. The PL spectrum of **2** consists of three bands in the NIR region corresponding to $^4F_{3/2} \rightarrow {}^4I_{9/2}$ (900 nm), $^4I_{11/2}$ (1063 nm), $^4I_{13/2}$ (1380 nm) electronic transitions inside the Nd^{3+} ion. NIR emission of **2** was found to be much stronger than that of $NdCl_3$ due to the ligand to metal energy transfer. As Zn^{2+} ion activates yellow fluorescence of the deprotonated form of salen ligand it was reasonable to examine whether complex **1** coordinated to Nd^{3+} ion can facilitate the energy transfer from the chromophore salen group to the lanthanide atom. It has been found that NIR emission intensity for **3** is practically two times higher than that for **2**. In the meanwhile, we observed notably reduced fluorescence from zinc chromophore for **3** with respect to compound **1** which is in line with Förster energy transfer phenomenon.

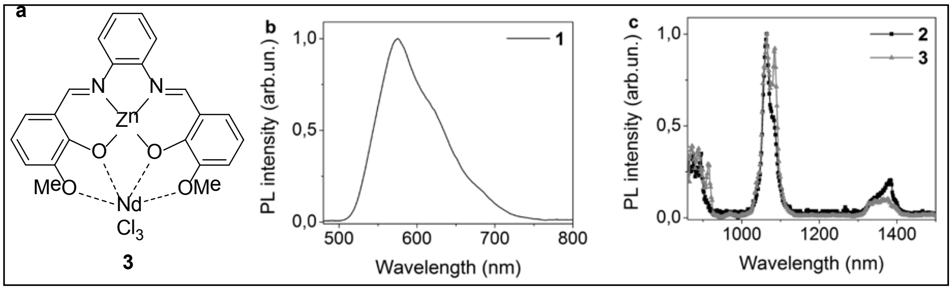

Fig. 1. Structure of the complex **3** (a), fluorescence spectrum of **1** (b), and NIR emission of **2** and **3** (c).

This work was supported by RFBR (project № 16-33-00056).

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P-36

Development of nanoscale contacts for organization and study low-molecular channel OFET

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The recent results on the formation of transistor structures indicate that the increase in the structuring of layers and orientation of molecules by improving the film deposition techniques leads to a significant improvement of the carrier mobility up to 40 $cm^2/V \cdot s$[1]. On the other hand, in the case of forming a nanoscale contacts a further improvement in mobility potentially can be expected due to preserving crystalline structure of material at sizes ~20-100 nm[2]. The study of transport mechanisms of high-structured molecular channel and field effect can be provided in lateral nano-gap. This requires the formation of nanoscale contacts at sufficiently reproducible manner, including size of gap, quality of contacts, for which etching carbon nanotubes (CNTs) and their bundles were used. CNTs deposited[3] on the initial substrate, and than formation of metal contacts to them by photolithography with a distance of 2 um was carried out. Then, local etching was carried out by a focused ion beam (FIB) Ga^+ at 30 pA and 1 pA current with different doses. When using bundles of 2-4 CNT likely metal type nano-contacts formed, that is optimal for the investigation of transport of certain molecules and their small groups, which after etching the CNT may be deposited into the gap. It was determined that size of the created gap is about 20-30 nm, and for CNT bundles substantially less than 20 nm, while the absence of conductivity and with a gap not visualize in SEM, because of the effects of the charge around the CNT (fig. 1a). As a result of the etching of CNT by FIB significant features were found in the etching of SiO_2, and the CNTs. The dose required for etching the CNT, which ~ $1.1 \cdot 10^{16}$ cm^{-2}, resulted in dielectric etching to a depth greater than the diameter of the CNT by 25-50% (Fig. 1b). To reduce the gap, depth and height of the boundary SiO_2 etching effects, for a part of the structures two-pass technique of etching CNT with pre-etched region modification of CNT with a dose ~ $7 \cdot 10^{14}$ cm^{-2} was carried out. These create differences in electric contact to molecular channel, and can be used to determine the contribution of contacts in charge transport. Significant field in nano-gap generates efficient charge injection into the channel that impact to creation the structure with low-conductive and conductive polymer molecules without doping, which are poorly investigated in view of studies materials having a good conductivity at macro level.

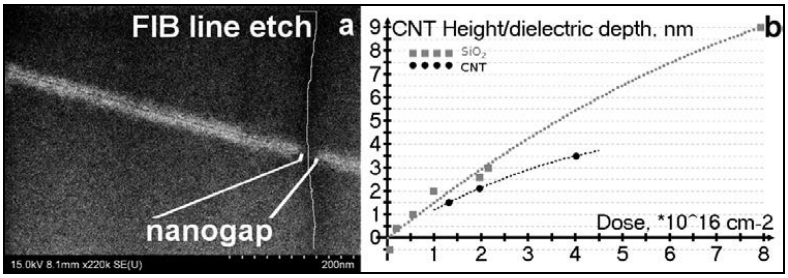

Fig. 1. a – typical gap, formed by etching, (SEM, bar with dashes is 200 nm); b – the dose of FIB at a current of 30 pA, for etching depth in the SiO_2 and CNTs with different diameters.

This work was supported by the Russian Science Foundation (project № 14-19-01308, MIET).

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P-37

Role of energetic disorder and traps on exciton lifetime in conjugated polymers

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By performing time-resolved photoluminescence (TRPL) spectroscopy on thin polymer films, we investigated the exciton lifetime in a whole range of conjugated polymers in dependence of their energetic disorder including poly(*p*-phenylene vinylene) (PPV)−based derivatives. We found that polymers with less energetic disorder exhibit an almost single exponential PL decay with decay times (exciton lifetime) of a few hundred picoseconds. In contrast, polymers with a large degree of disorder show non-monoexponential PL decays and a relatively longer exciton lifetime in the nanosecond range. Remarkably, a disorder independent exciton diffusion length of about 5–7 nm is found. Assuming that the PL decay time in neat polymer film is not determined by the intrinsic exciton lifetime, but by the diffusion-limited exciton quenching at non-radiative recombination centers that are present in organic semiconductors, the measured PL decay time reflects the time that excitons need to diffuse towards these quenching sites. Therefore, the short PL decay times in better ordered materials is ascribed to fast exciton diffusion towards trap-sites relative to slower diffusion in more disordered polymers. From TRPL measurements, using randomly distributed fullerene quenchers, we demonstrate that the background concentration of exciton quenching defects in pristine polymer films is nearly the same as the universal electron trap concentration of typically 10^{17}–10^{18} cm^{-3}.[1,2] This observation strongly suggests that the exciton quenching defects and the electron traps share the same origin. Considering that there is a universal amount of non-radiative quenchers in a wide range of organic semiconductors provides an explanation why different materials have a similar exciton diffusion length of 5–7 nm, in spite of a large variation in exciton lifetime (diffusion coefficient).

This work was supported by DPI (project № 763).

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P-38

Effect of microscopic Coulomb interactions on the mobility of charge carriers in disordered organics

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Transport in organic materials occurs due to hopping of charge carriers between localized states, randomly distributed in energy. The mobility of charge carriers is one of the most important characteristics of transport. It was shown both experimentally[1] and theoretically[2], that the mobility is increasing significantly with increasing concentration. The filling of deep states is considered to be the main reason of this effect. In that case these states stop acting as “traps”. However, at moderate concentrations the other effect could be more significant – strong Coulomb repulsion of randomly nearing charges, which accelerates the release of charges from deep states. In a present work the distribution function of the module of Coulomb field, created by the nearest neighboring charge, was obtained. Concentration dependence of mobility is calculated by averaging of «local» mobility, which corresponds to the certain value of this field. The «local» mobility was calculated according to percolation approach with the use of effective transport energy concept[3], which is seemingly valid also in the case of correlated disorder[4]: $\mu\left(F,c\right)=\frac{\mu_0}{c}\exp\left[-\frac{E_C(F)-E_F\left(c\right)}{kT}\right]$, where $E_C(F)=E_{C0}+kT\varphi\sqrt{F}$, $\varphi=\tilde{C}\left[\left(\sigma/kT\right)^{3/2}-\Gamma\right]$ – the effective transport energy, E_F – quasi-Fermi energy.

One should consider three main factors, which affect the mobility of charge carriers in disordered organic materials: energetic and position disorder, microscopic Coulomb interactions of neighboring charges and energetic-spatial correlations due to charge-dipole interactions[5]. These correlations result in a potential well around rather deep states, which controls the mobility. Monte-Carlo modelling shows that this potential well is rather good described by Coulomb-type function, $W(r)\sim-\alpha/r$, where r is a distance from the initial deep state. In the present work we consider a charge, trying to escape from the potential well, created by all of these factors in the presence of external electric field. Coulomb repulsion leads to the reduction of a potential barrier, as well as the external field. This approach leads to field dependence of mobility in well-known Pool-Frenkel form, which could be presented also as field dependence of transport energy, mentioned above. Results show, that the effect of field dependence of transport level on mobility is no less significant, than the filling of deep states, in accord with known results of Monte-Carlo simulations[v].

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P-39

Di(benzothieno)thiazines – New Electron Rich Organic Molecules

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Di(benzothieno)thiazines represent a new class of electron rich organic π-systems. They share structural similarities with phenothiazines[1] and dithienothiazines[2] due to their central thiazine core. All these systems adopt butterfly conformations of the nonaromatic central ring. After oxidation radical cations are generated, which are fully delocalized over the now planar π-systems. This accounts for the excellent electronic properties of phenothiazines and dithienothiazines. Di(benzothieno)thiazines display similar electronic properties, such as low oxidation potentials and two reversible oxidation processes (Fig. 1), even more favorable than phenothiazines in this regard.

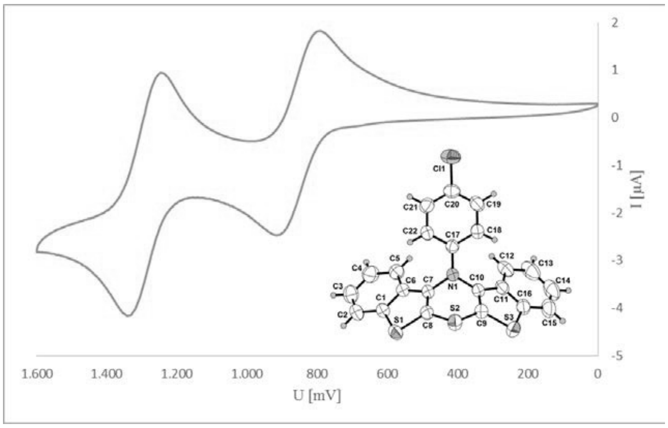

Fig. 1 Cyclic voltammogram of a di(benzothieno)thiazine

Di(benzothieno)thiazines can be synthesized by inter-intramolecular *Buchwald-Hartwig* coupling of bis(3-bromobenzo[b]thiophen-2-yl)sulfane with the corresponding amine (Fig. 2).

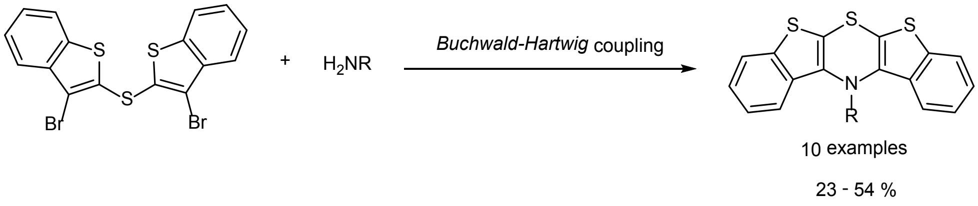

Fig. 2 Synthesis of di(benzothieno)thiazines.

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P-40

Kinetic Modeling of PPV Polymerization via Gilch

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Poly(p-phenylene vinylene)s (PPVs) are widely used polymers for application in organic electronic devices and are promising materials for bioimaging nowadays.[1] The most efficient synthetic approach towards high molecular weight PPVs is the Gilch (precursor-) route. Treating α,α′-dibromo-p-xylenes with a strong base initiates a cascade of reactions leading to the conjugated PPVs (see inset Figure 1). The complexity of this reaction network may well explain the often encountered and undesired batch-to-batch variations in opto-electrical performance. Schwalm *et al.* studied the Gilch polymerization using ^{1}H-NMR spectroscopy and qualitatively indicated the species involved in the various reaction steps. They identified quinodimethane **2** as the active monomer. Unfortunately, this study did not provide quantitative kinetic information.[2,3] We investigated the reaction cascade of poly(2,5-bis-(2′-ethyl-hexyl)-1,4-phenylenevinylene) (BEH-PPV) using time-resolved ^{1}H-NMR spectros-copy and developed an extended fitting model describing the kinetics of all individual reaction steps in the synthesis of BEH-PPV (see Figure 1). By fitting this model to our experimental data we not only derived rate constants for monomer consumption and polymerization, but also for the final elimination step towards the conjugated end product.

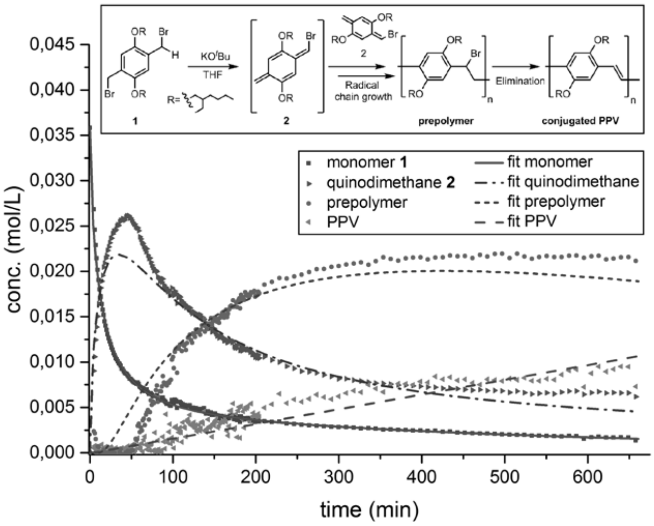

Figure 1: Measured concentrations and corresponding fits respecively: monomer **1** (square; solid line), quinodimethane **2** (right triangle; dash dot), prepolymer (circle; dot) and PPV (left triangle; dashed). The inset shows the reduced reaction cascade from monomer **1** to PPV.

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P-41

Synthesis, optical and electrochemical properties of new π-conjugated systems, containing prop-2-en-1-one, 2-aminopyrimidine and 2-(1H-pyrrol-1-yl)pyrimidine moieties

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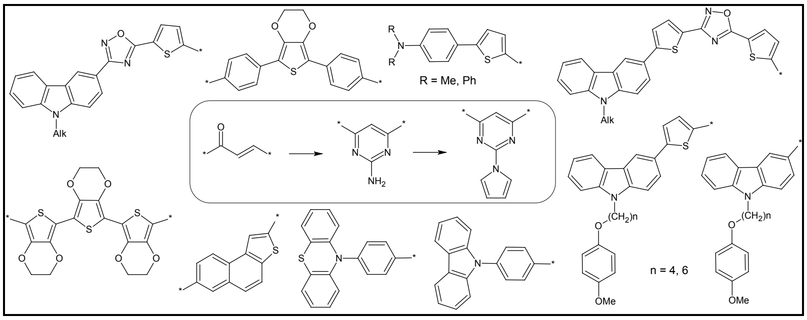
Nowadays a large amount of research going on in the field of organic electronics are devoted to the molecular design and synthesis of new compounds the main feature of which is the presence of a prolongated conjugated system in their structures[1]. Such kind of compounds have been found to increase the efficiency of electronic devices based on them. A keynote principle of this work consists in the introduction into the structure of a future organic molecule simultaneously electron deficient (A) and electron excessive (D) fragments. As a results there can be prepared various conjugated systems of D-A-D, A-D-A, D-π-A, D-A-D-A-D or A-D-A-D-A type. Compounds of such structure are characterized by an efficient intramolecular charge transfer, which provides the decrease in a bandgap values and the improvement of transport and photovoltaic properties[2]. Here we present the synthetic procedure and investigation of new the π-conjugated systems including prop-2-en-1-one, 2-aminopyrimidine or 2-(1H-pyrrol-1-yl)pyrimidine moieties as electron deficient cores. Triphenylamine, N-alkylcarbazole, phenothiazine, 3,4-ethylenedioxythiophene and naphto[2,1-*b*]thiophene were incorporated as electron donor fragments in the structure of these compounds. The nature, the number and the sequence of these heterocycles allow to tune the optical and electrochemical properties of a future compound.



Electronic absorption and fluorescence spectra as well as electrochemical properties have been studied for all the prepared compounds. Some compounds were found to have good film forming properties that gave the possibility to prepared thin films, which fine structures had been examined by scanning tunneling microscopy NTegro – Prima.

The work was financially supported by the Ministry of Education and Science of the RF (project N 012011461916) and by RFBR (projects N 14-03-00341a, 14-03-96003_Ural-a). Instrumental studies were performed with the help of equipment purchased at the expense of the Program of National Research Universities of RF (Perm State University).

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Electrical characterization of self-assembled monolayer field-effect transistors based on Langmuir films of organosilicon conjugated oligomers

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Organic Field-Effect Transistor (OFET) is one of the main building blocks of low-cost organic electronics. Monolayer OFETs is an object of growing scientific interest because low semiconductor thickness provides high sensitivity to the media, which makes them perspective in different sensing applications. A traditional approach to the fabrication of monolayer OFETs is a self-assembly from the solution on the substrate. However, this process involves formation of the covalent bonds between the semiconducting film and the dielectric. For this purpose, self-assembly requires chemically active molecules (e.g. chlorosilanes), which are not chemically stable in an air environment. In addition, the process of layer formation is relatively slow (tens of hours for full surface coverage).

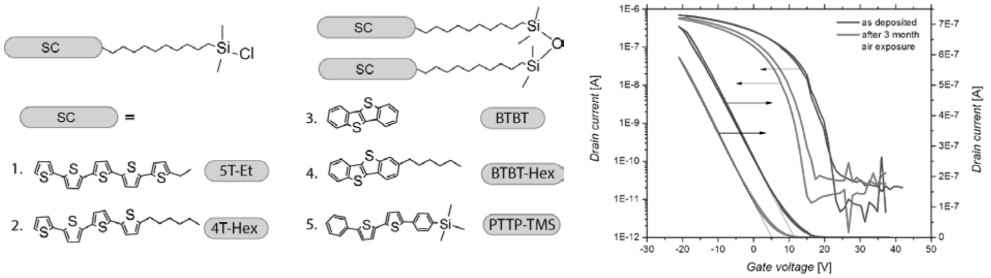

Fig. 1. Chemical structure of organic semiconductors (a) and transfer characteristics of monolayer LB OFET with 30-μm channel length on the base of O(Si-Und-4T-Hex)$_2$ (b).

In this work, we apply Langmuir-Blodgett (LB) and Langmuir-Schaefer (LS) techniques to the fabrication of self-assembled monolayer OFETs (SAMFETs) based on a series of reactive (chlorosilane) and chemically inert (disiloxane) derivatives of oligothiophenes, [1]benzothieno[3,2-b][1]-benzothiophene (BTBT) and thiophene-phenylene (PTTP) (see Fig. 1a). Efficient SAMFETs with charge carrier mobilities up to 0.01 cm^2/Vs and on/off ratio up to 10^6 were fabricated. The performance of SAMFETs reported is close to those of the SAMFETs prepared by self-assembly from solution. Typical transfer curves of the monolayer LB OFETs with 30-μm channel length based on disiloxane dimer O(Si-Und-4T-Hex)$_2$ are shown in Fig. 1b.[1] Fabricated OFETs demonstrated high reproducibility and stability under normal conditions.[2] The developed approach can be utilized in large-area low-cost electronics production, such as gas sensor applications.

This work was supported by RFBR (grant 14-03-00873) and Russian Academy of Sciences (program P-1).

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New nanostructured organosilicon luminophores for organic photonics

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During the last years a number of light-harvesting luminescent dendrimers has increased rapidly[1]. One of the most interesting features of dendrimers is a possibility of incorporation of different chromophores within one nanostructured dendritic molecule that lead to an intramolecular directional energy transfer from their external chromophores to the center (the so called "molecular antenna effect"). It allows tuning the emission color of the core across the entire visible spectrum, which provides an efficient tool for controlling a wavelength of light emission in organic photonic and electronic devices. Recently we have reported first organosilicon molecular antennas, which contained non-functional alkyl groups[2-4]. However, their luminescence efficiencies were rather low.

In this work we synthesized a number new organosilicon molecular antennas with phenyloxazole fragments: 2,5-diphenyl-1,3-oxazole (PPO) and 1,4-bis(5-phenyl-2-oxazolyl)benzene (POPOP), an example of which is shown on Fig. 1. These phenyloxazoles are well known for their highly efficient emission in UV and blue spectral regions, respectively, and high Stokes shift values. They possess large absorption cross-section and high luminescent quantum yield.

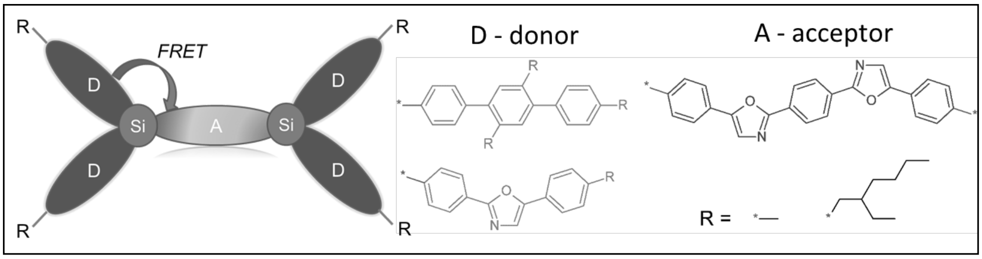

Fig. 1. Chemical structure of representative nanostructured organosilicon luminophores.

Photoluminescence study of the new molecules has shown an intramolecular energy transfer with the efficiency up to 99% and luminescence quantum yield up to 97% with the emission maximum at 425 nm indepentantly on the type of peripieral donor fragments. Both oligoarylsilanes have high extinction coefficients up to 290 000 $M^{-1}cm^{-1}$ and good solubility in common organic solvents. These properties allow to attribute them to a novel class of highly efficient luminescent materials called as nanostructured organisilicon luminophores (NOLs).[5] They have a high potential for application as functional materials in solution-processilble organic light-emitting diodes (OLEDs) and UV-Vis wavelength shifters.

This work was supported by Russian Foundation for Basic Research (№ 16-33-01100)

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P-44

Novel donor-acceptor oligomers of different architecture based on triphenylamine and carbazole for organic photovoltaics

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Triphenylamine (TPA) derivatives are well known photoconducting materials with high hole mobility. TPA-derivatives have been widely investigated as promising materials for organic electronics[1]. Recently a number of star-shaped molecules based on TPA and containing oligothiophene as π-bridges and alkyldycianovinyl groups as acceptor units have been synthesized[2, 3, 4]. These star-shaped molecules have been widely investigated as one of the most promising materials for organic photovoltaics. However, there is a need to optimize photophysical properties of TPA-based oligomers. In this work, TPA core was modified using carbazole, which is more planar analog of TPA. Also, this work shows the synthesis of a series of oligomers having novel electron donating tris(2-methoxyphenyl)amine core and novel acceptor units – 3-ethylrhodanine groups[5]. Besides, we demonstrate series of push-pull unsymmetrical oligomers based on electron-donating TPA and electron-withdrawing dicyanovinyl group.

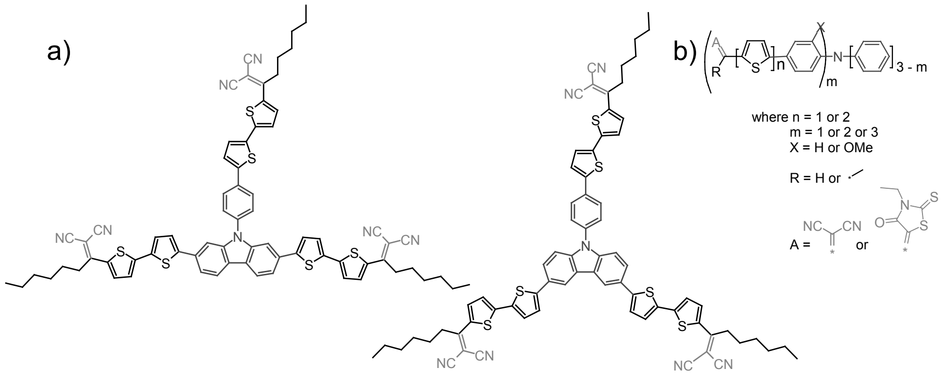

Fig. 1. Schematic representation of star-shaped carbazole-based oligomers (a) and oligomers based on triphenylamine.

Variations of parameters of their chemical structures such as type of acceptor and donor groups were used to study the structure-properties relationships in this new type of molecules.

This work was supported by Russian Foundation for Basic Research (grant 16-33-01123). The work in the part of synthesis and investigations of star-shaped oligomers was supported by Russian Science Foundation (14-13-01380).

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P-45

Relation between supramolecular structure and the charge and excited state dynamics in organic materials

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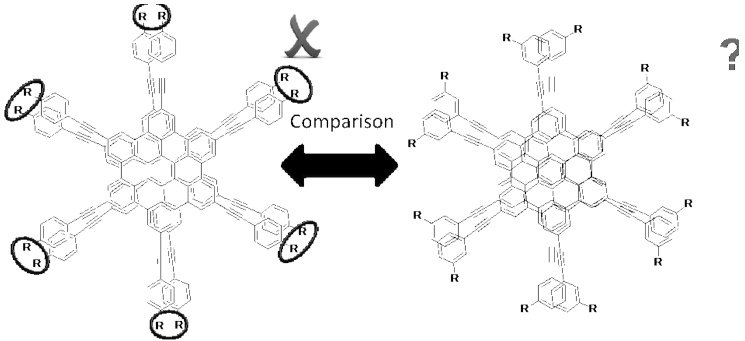

1 2

Figure 1. Steric hindrance effect by specific side chains

This study aims to achieve control over charge and excited state dynamics by engineering the optoelectronic properties of new organic semiconductor molecules and the way they organize in the solid state. HBCs have been studied extensively in the past and soluble alkyl-substituted derivatives of HBC exhibit some of the highest intrinsic charge carrier mobilities.[1,2] Due to the steric hindrance of the side chains, there is typically a substantial rotation of neighboring molecules with respect to each other which is 30 degrees for HBCs. Interestingly, when the charge transfer integral between neighboring molecules is considered by density functional theory calculations, it becomes clear that this is the least favorable conformation for charge and exciton transport.[3,4] In this work, we aim to reduce the steric hindrance by specific side chains where the aliphatic solubilizing substituents are placed in a meta configuration as shown in Figure 1. This leads to considerable differences in the supramolecular organization, as shown by XRD and solid state NMR. It is shown that this changed supramolecular organization results in interesting changes in the electronic properties, for instance the mobility of charges.

This work is supported by ERC Consolidator Grant (Project number TFHB78)

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Unsymmetrical push-pull oligomers based on triphenylamine: synthesis and properties

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Donor-acceptor oligomers based on electron-donating triphenylamine and electron-withdrawing dicyanovinyl groups are actively researched as promising semiconductor materials for organic photovoltaics [1, 2, 3, 4, 5]. In this work novel unsymmetrical donor-acceptor oligomers based on the triphenylamine with oligothiophene arms end-capped with dicyanovinyl substituent were synthesized, investigated and compared to each other (Figure 1). The unsymmetrical molecules have a low molecular weight which makes possible using vacuum sublimation technique for fabrication of organic solar cells. Besides, their synthesis is more convenient. Synthesis of the unsymmetrical donor-acceptor oligomers based on a recently developed synthetic approach using the Knövenagel condensation under a microwave irradiation[6]. The electrochemical, thermal and optical properties of molecules were investigated by cyclic voltammetry, differential scanning calorimetry, thermogravimetric analysis and UV-Vis spectroscopy. Properties of these oligomers will be compared to each other.

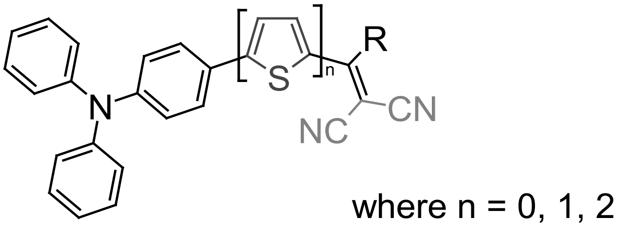

Fig. 1. Schematic representation of unsymmetrical oligomers.

This work was supported by Russian Foundation for Basic Research (grants 16-33-01123)

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P-47

Modeling of the photocurrent in organic field-effect transistors

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Organic field-effect transistors (OFET) can combine photodetection and light amplification, i.e. work as phototransistors. Such organic phototransistors can be used in light-controlled switches and amplifiers, detection circuits, and sensors of ultrasensitive images[1]. The main components of the OFET structure are shown in Fig 1a.

In this work, we propose a simple one-dimensional numerical model of photosensitive OFET. The model is based on the Poisson, current continuity and drift-diffusion equations with one spatial coordinate directed in plane of the active layer from source to drain electrode. The model allows calculation the dependences of the source-drain current on the source-drain voltage V_d (output characteristics) and on the gate voltage V_g (transfer characteristics). Fig. 1b shows the photocurrent versus V_g (difference between calculated transfer characteristics upon light and in dark) for OFET with p-channel when the Fermi levels of the source and drain electrodes aligned to the highest occupied molecular orbital of the organic semiconductor.

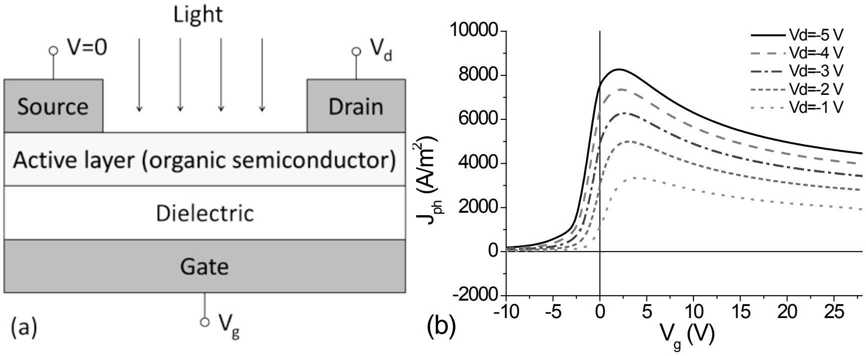

Fig. 1. Scheme of OFET (a) and dependence of photocurrent density J_{ph} on V_g at different V_d for p-channel OFET (b).

As shown in Fig. 1b, there is an optimal value of V_g near 2 V at which the photocurrent is maximal. We figured out that these V_g-dependences of the photocurrent result from variation in the area of efficient charge photogeneration. At $V_g<0$, the photogeneration of electron-hole pairs is compensated by their recombination in the whole active layer; therefore, the photocurrent tends to zero. At optimal V_g near 2 V, the hole-depleted area is formed near the drain electrode, where the electric field is enhanced and charge recombination suppressed. At higher V_g this area narrows, and J_{ph} decreases. The model shows that the photosensitivity (photocurrent to dark current ratio) at optimal V_g is higher than 10^{10}. We have studied effects of different OFET parameters such as band gap, charge mobility, channel length, etc. on the photocurrent. We compare the results of modeling with the experimental data.

This work was supported by RFBR (project № 15-53-10070).

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P-48

Highly stable ultrathin OFETs from siloxane dimers of BTBT

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The most part of organic electronic devices is based on organic field-effect transistors (OFETs). One of the perspective pathways in organic electronic is development of ultrathin OFETs because the charge transport within the OFET mainly takes place in one-two molecular layers of organic semiconductor[1]. However, such devices usually demonstrate lower performance because of too much defects in active monolayer films.

Here we adopted spin-coating (SC), Langmuir-Blodgett (LB) and Langmuir-Schaefer (LS) techniques for formation of low-defect organic semiconductor ultrathin films and used them as active layers in OFETs. Disiloxane dimers of BTBT – 1,3-*bis*[11-(7-hexyl[1] benzothieno[3,2-b][1]benzothien-2-yl)undecyl]-1,1,3,3-tetramethyldisiloxane, **O-(Si-Und-BTBT-Hex)$_2$** and 1,3-bis(11-[1]benzothieno[3,2-b][1]benzothien-2-yl-undecyl)-1,1,3,3-tetramethyldisiloxane, **O-(Si-Und-BTBT)$_2$** have been chosen for this purpose by several reasons – impressive electrical performance of dialkyl derivatives of the semiconductor core – BTBT (up to 43 cm^2/(Vs) for thick OFETs[2]); high air-stability of the semiconductor core[3]; and possibility of using Langmuir techniques for the monolayer formation due to presence of disiloxane fragment into the molecular structure of these dimers[4]. For achieving low-defect ultrathin films, we investigated three alternative ways: surface modification of a substrate; variation of the semiconductor concentration; variation of the processing conditions. Figure 1 demonstrates AFM images of monolayer films based on dimers (a,b) obtained by SC technique at optimal conditions and typical transfer characteristics of OTFTs based on these films with 30 μm channel length.

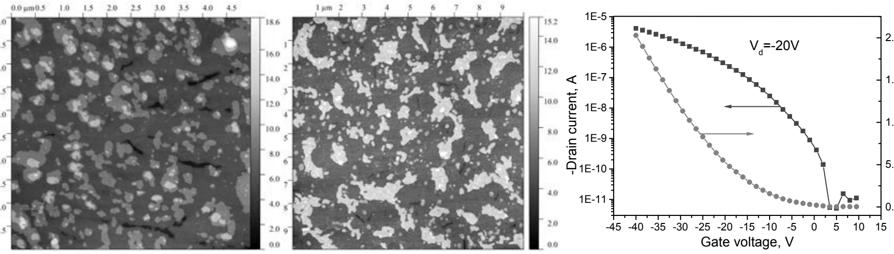

Figure 1. AFM images of spin-coated film of **O-(Si-Und-BTBT-Hex)$_2$** (a) and **O-(Si-Und-BTBT)$_2$** (b), obtained at optimal conditions. (c) Typical transfer characteristics of OTEFs.

The linear and saturated hole mobilities were found to be in the range of 10^{-5}-10^{-2} cm^2/Vs depending in the preparation conditions. It was found that the presence of terminal aliphatic groups (-**Hex**) is crucial for the device performance. The best characteristics were obtained for the devices based on **O-(Si-Und-BTBT-Hex)$_2$** by SC technique: charge carrier mobility of 4×10^{-2} cm^2/Vs and on/off current ratio of 10^6. OTFTs prepared were found to be stable at least after half a year storage under ambient conditions that enables using this dimer for large-area electronics production.

This work was supported by RFBR (projects № 14-03-00873 and 16-29-05321).

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Singlet fission in pentacene solar cells

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Recently, organic solar cells with efficiencies over 10% were reported. In theory, however, efficiencies up to 20% were predicted.[1] A promising way of beating this limit is via singlet fission, a spin-allowed process in which two molecules of which one is in a singlet excited state (S_1), distribute their energies to give to molecules with a triplet excited state (T_1).[2] For this process to be energetically allowed, the T_1 state energy can be at maximum half the S_1 state energy. In the end this results in an increased current by decreasing the open-circuit voltage V_{OC} of the solar cell.

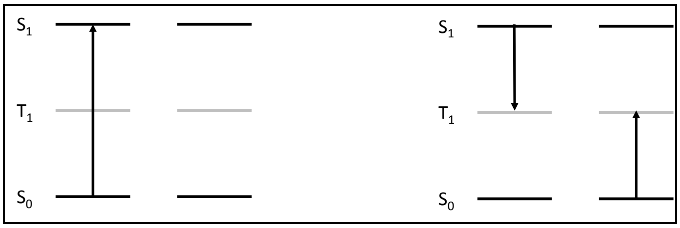

Fig. 1. The singlet fission process: first, excitation from S_0 to S_1 (left) and, subsequently, distribution of the energy to two T_1 states (right).

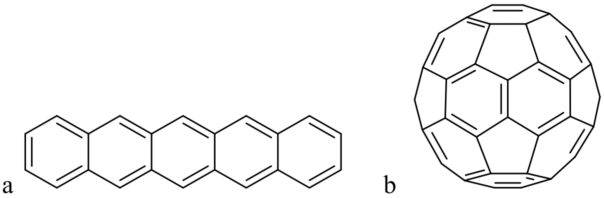

Fig. 2. The chemical structures of pentacene (a) and fullerene C_{60} (b).

A typical material to undergo singlet fission is pentacene. Congreve *et al.* showed that in bilayer solar cells with fullerene C_{60} as electron acceptor, an external quantum efficiency (EQE) of over 100% was reached, indicating one photon can generate more than one electron.[3] Another way of studying singlet fission is via spectroscopic techniques.

Pentacene bilayer solar cells with four different acceptors were fabricated in order to study the effect of the acceptor on the solar cell performance. The obtained open-circuit potential V_{OC} clearly increases with the E_{vac} of the fullerene chosen as acceptor, where there is a sharp drop in short-circuit current density J_{SC}, even for cells with an E_{vac} more than 0.6 eV[4] below the singlet energy of pentacene. This shows that singlet fission plays an important role in pentacene:fullerene solar cells.

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Oxygen contents and the surface workfunction of the liquid phase deposited graphene oxide films studied by photoelectron spectroscopy

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The atomic composition of conjugated organic films, possible interfacial reactions and interfacial dipole layer formation can well be studied using X-ray photoelectron spectroscopy (XPS) and the ultraviolet photoelectron spectroscopy (UPS)[1,2]. Graphene oxide (GO) has been found to be a promising component of the organic-inorganic composite materials for the purposes of the photovoltaic, field effect transistor and electronic switching device applications[3]. In the present study the atomic composition poly(9-vinylcarbazole)/GO (PVC/GO) blends at room temperatures and at moderate heating about 80 ºC was measured. The contents of the main atomic components of the *ex situ* prepared PVC/GO corresponds approximately to the chemical formulas of the compounds studied. However the relative contents of the contaminations adsorbed from the atmosphere was estimated as 15-25%. For the detailed analysis the thin GO films were deposited onto the tantalum (Ta) surface and subjected to the series of the XPS and UPS tests under the two surface treatment procedures: the Ar+ ion bombardment cleaning and heating up to 800 ºC. Both types of the surface treatment showed the possibility of removing of the atmospheric contamination adsorbates while keeping the GO material intact. There was possible to distinguish the oxygen within the Ta oxide substrate and within the GO film. The UPS results showed a relatively smeared peak structure of the GO valence band while it was possible to detect the energy position of the Fermi level in the Ta substrate and the location of the valence band edge (HOMO) of the GO film.

The measurements were performed at the Center for Studies in Surface Science of Research park of St.Petersburg State University, the support from RFBR grant 14-03-00087 and from the St.Petersburg State University research grant 11.38.219.2014 is greatly appreciated.

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Conduction band electronic structure of the ultrathin films of substituted perylene and fullerene on germanium oxide surface

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Thin films structures made from substituted perylene films on oxidized germanium ((GeO$_2$)Ge) surface attract scientific interest due to their possible application in organic electronics devices[1]. C$_{60}$ end-capping of the conjugated molecules may be used for anchoring of the molecules to the electrodes and for the design of the molecular wires[2]. In the present study the surface work function and the density of the unoccupied electron states (DOUS) located 5-20 eV above the Fermi level (E$_F$) were investigated during the deposition of the dioctyl-substituted and diphenyl-substituted perylene dicarboxyimide (PTCDI-C$_8$ and PTCDI-Ph) as well as fullerene substituted benzene onto the (GeO$_2$)Ge surface. Experimentally, the total electron yield resulted from incident electron beam of 0-30 eV interacting with the sample surface was measured using the total current spectroscopy (TCS) technique. The TCS peak position in the cases of the PTCDI-C$_8$ and PTCDI-Ph differs mostly in the electron energy range from 9 eV to 20 eV above E$_F$. The electron energy range affected by the benzene bonding to the C$_{60}$ was found to be between 6 eV and 10 eV above the E$_F$ and both π*- and σ*- type orbitals were affected by adding the substituents. The 0.1-0.3 eV changes of the workfunction values were observed as a result of the deposition of the 5-10 nm thick organic overlayers studied onto the (GeO$_2$)Ge substrate surface, which characterizes the electronic charge transfer at the interfaces.

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Energy level alignment in the ultra-thin layers of polar substituted phthalocyanine and phenylene-vinylene oligomer on solid substrate

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The energy level alignment and the peak structure of the density of the valence and of the unoccupied electronic states (DOS and DOUS, respectively) in organic interfacial structures is a subject of a great scientific interest due to the possible electronic device applications. Introducing polar substituents into the molecules can be used to tune the electronic structure of the organic materials[1].

In the present work the potential barrier formation and the DOUS were studied at the interfaces of the hexadecafluoro copper phthalocyanine (F_{16}-CuPc), unsubstituted CuPc, the dinitro substituted phenylene-vinylene oligomer (NO_2-OPV) and unsubstituted OPV ultrathin films deposited on the surface of oxidized Si and of binary semiconductor substrates. The experimental results were obtained by monitoring secondary electrons backscattered from the sample surface. The total electron yield resulted from incident electron beam of 0-30 eV interacting with the sample surface was measured using the total current spectroscopy (TCS) technique. The assignment of the DOUS peaks obtained from the experiments was made using the density functional theory (DFT) calculations.

The substantial changes of the DOUS peak structure in the π^* and the low-lying σ^* region were observed at the interface region between the ultrathin layers of the unsubstituted CuPc and OPV films and the substituted ones, F_{16}-CuPc and NO_2-OPV, respectively[2]. The energy level alignment was accompanied by the interfacial charge transfer and by the formation of the approximately 2 nm thick polarization layer in the organic films. Among other electronic processes which occur at the interfaces the formation of the 1-2 nm thick intermediate layer of the fragmented overlayer molecules on some of the surfaces of the semiconductors.

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Density of the unoccupied electronic states of the films of dioctyl-substituted and of diphenyl-substituted perylenedicarboximide

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Modification of electronic properties of organic semiconducting materials is an attractive problem due to a large potential of these materials to be a component of organic electronic devices[1]. One of possibilities to improve characteristics of these devices is to use substituent groups on molecules. So dioctyl-substituted (-C_8) and diphenyl-substituted (-Ph) perylenedicarboximide (PTCDI) are considered as perspective materials. The use of substituent groups transforms density of electronic states of organic molecules under study and changes their electronic properties.

We present the results of the experimental studies of the density of unoccupied electronic states (DOUS) as well as the results of the theoretical calculations based on the density functional theory obtained for the ultrathin films of substituted perylenes. Experimentally, the total current spectroscopy and the dissociative electron attachment methods were applied, which use the low energy electron beam as a testing probe for the surface under study. The calculation method used the B3LYP functional and a standard 6-31G(d) basis set. The comparison of the DOUS of PTCDI, PTCDI-C_8 and PTCDI-Ph films obtained with both experimental and theoretical methods is presented. The π^* orbitals band of PTCDI-C_8 and PTCDI-Ph detected over the range 2 to 8 eV. π^* maxima of PTCDI-Ph are less energetic by 0,5-1 eV then π^* maxima of PTCDI-C_8.The mix orbitals band of PTCDI-C_8 and PTCDI-Ph detected over the range 8 to 10 eV. The σ^* orbitals band of PTCDI-C_8 and PTCDI-Ph begins at 10 eV. σ^* maxima of both molecules differ slightly especially over the ranges 10 to 15 eV. The interaction of the low-energy electrons with the PTCDI sampls in the gas phase and in the solid phase is discussed in terms of possible relation to the biochemical reactions of electron attachment which occur in liquid phase[2,3].

The work was supported by the St. Petersburg State University research grant 11.38.219.2014 and by the RFBR grants 14-03-00087 and 15-29-05786.

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Structure and magnetic properties of nanocrystalline mechanically alloyed Fe-10%Zn and Fe-30%Zn

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Nanocrystalline Fe-10%Zn and Fe-30%Zn alloys have been prepared from pure elemental powders by mechanical alloying processing in a high energy planetary ball-mill. Morphological, microstructural, structural, and magnetic characterizations of the powders were investigated by scanning electron microscopy, X-ray diffraction, and vibrating sample magnometer. The crystallite size reduction to the nanometer scale is accompanied by an increase in the atomic level strain. The reaction between Fe and Zn leads to the formation of a solid solution bcc-Fe(Zn) with a lattice parameter close to 0.2910 nm for Fe-30%Zn and 0.2885 nm for Fe-10%Zn, after 24 h of milling. The complete dissolution of the elemental Zn powders in the α-Fe lattice gives rise to the formation of a solid solution Fe(Zn), where α-Fe(Zn) nanograins have a crystallite size of 22.92 nm for Fe-10%Zn and 30.09 nm for Fe-30%Zn, on prolonged milling time. The coercivity values are 18.90 Oe and 26.59 Oe for Fe-10%Zn, Fe-30%Zn, respectively, after 24 h of milling.

Molecular dynamics simulation of P3HT helical structure in vacuo and in amorphous polymer surrounding

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Recently, composites based on conjugated polymers filled with carbon nanoparticles have been applied extensively in the field of organic electronics. Regioregular poly-3-hexylthiophene (P3HT) is polyconjugated heterocyclic polymer commonly used as an electron donor material in such composites. The efficiency of organic photovoltaic cells made of P3HT-based composites essentially depends on the structure of polymer matrix within the interface region between components. This is due to the fact that both polymer-donor and acceptor materials must provide ‘a continuous path’ for electron and hole transport to the respective electrodes to ensure efficient photocurrent generation. P3HT is a semicrystalline polymer and its structure is usually described as a combination of crystalline and amorphous domains. The most common representation of the P3HT crystalline domain structure is believed to be layers of parallel P3HT chains in elongated conformation. However, Kiriy *et al.*[1] suggested the potential existence of the helical conformation of P3HT chains.

With a view to determine whether P3HT can exist in a helical conformation, the potential impact of amorphous polymer surrounding, electrostatic interactions and temperature regime on structure evolution of a single P3HT chain in a helical conformation is investigated via molecular dynamics simulations using the GROMACS software package. The interactions in the systems under investigation are described by Gromos53a5 or Amber99sb force fields. Partial charges for P3HT atoms are calculated using quantum-chemical methods. The initial helical conformation of a P3HT chain in all anti conformation is generated with degree of polymerization $N_p = 70$. The energy of the initial chain configuration is minimized by means of molecular mechanics. First, simulation of the box containing one P3HT chain in a helical conformation in vacuo is performed without electrostatic interactions at three temperatures (room temperature, below and sufficienty higher the P3HT melting point) in order to determine its stability and possible structure evolution. Then, simulation of helical structure in amorphous polymer surrounding is carried out at the above-mentioned temperatures both with and without electrostatic interactions. According to the study, when using Gromos force field the helical chain is stable in vacuo at room temperature, but it promptly loses its structure at elevated temperatures. The destruction of the structure in the presence of the amorphous surrounding took a significantly longer time when compared to the vacuo simulations. Thus, the amorphous surrounding is able to inhibit the destruction of the helical structure. The electrostatic interactions do not seem to substantially affect the stability of the P3HT helical structure. While using the Amber force field a ‘frozen’ structure is observed at temperature above the P3HT melting point, that indicates the necessity of further investigation.

This work was supported by the Russian Foundation for Basic Research (grant № 15-03-07614). The simulations were performed using the computational facilities of the Institute of Macromolecular Compounds, Russian Academy of Sciences, and the ‘Chebyshev’ and ‘Lomonosov’ supercomputers at Moscow State University.

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Computational rational design of cationic polyelectrolytes with enhanced hydrogen bonding ability for electrode buffer layers

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Due to their molecular structure, conjugated polyelectrolytes (CPEs) interact through pi-pi stacking, hydrophobic interactions, electrostatic forces and hydrogen bonding, and these interactions can be tuned by the surrounding media (e.g. solvent). In recent years different CPEs have been "revisited" to be tested as electrode selective "buffer" layers in organic optoelectronic devices, due to their interesting surface properties. As with many other materials, intuition- and serendipity-driven trial and error strategies had guided the synthesis of new CPEs. However, even when such "Edisonian" approach is undoubtedly powerful, useful and sometimes elegant,[1] it is highly experimentally demanding, and sometimes the results are not generalizable. In this regard, advanced computational screening offers a useful tool to generate basic knowledge and a reduced and targeted experimental synthesis.

This contribution presents our advances in a computational-based rational design of conjugated polyelectrolytes with enhanced hydrogen bonding ability for their use as buffer layers in organic solar cells, which is being performed by following a rational design strategy of hierarchical modelling with successive downselection stages. The first stage consists of a quantum mechanics-based combinatorial search to identify polymer repeating units that could lead to desirable dielectric properties, using density functional theory (DFT), which has been used for the screening of hydrogen-bonding molecules for organic optoelectronics,[2,3] monitoring dielectric constant, frontier molecular orbitals and band gap. These studies are performed using the B3LYP functional, which provides a relatively fast way to determine the electronic and optical properties of polymer systems.

In the second stage it will be performed a configurational space search using molecular dynamics (MD) to determine the three-dimensional (3D) arrangement of polymers (i.e. modes of aggregation) built from the desirable repeat units.[4] These studies will be performed using a single force field (GROMOS96 43A1), to perform an internal comparison, despite the possible errors associated to the use of this force field.

In terms of the molecules, the first stage consists of a 1D catenation of repeat units into a polymer chain, using mainly thiophene units functionalized with amine-related building blocks, since it has been observed experimentally, in organic solar cells, that when the amount of amine functionality in cathode buffer layers is reduced, the main device parameters (FF, Jsc and PCE) increase.[5] Also, some other molecules will be studied in order to contrast the results (e.g. polyethylene, polyesters, polyamides and polyethers). On the other hand, in the second stage, the intra- and inter-molecular aggregation of selected oligomers will be evaluated using explicit solvation, mainly in water.

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P-57

New D1-A-D2-A-D1-type Small Molecules Based on Fluorobenzotriazole Acceptor and Dithienosilole Core Donor for Solution Processed Organic Solar Cells

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Two small molecules denoted as **K2** and **K3** containing fluorine atoms at different positions of benzotriazole, with linear D1-A-D2-A-D1 configuration based on dithienosilole and fluorobenzotriazole as donor and acceptor materials, were designed and synthesized for small molecule organic solar cells. Their optical and electrochemical properties were investigated.

We have used these small molecules as electron donor along with the [6,6]-phenyl C60 butyric acid methyl ester or [6,6]-phenyl-C_{71}-butyric acid methyl ester as electron acceptor for the fabrication of solution processed organic bulk heterojunction solar cells. High power conversion efficiency values of 6.01% (J_{sc}=11.68 mA/cm^2, V_{oc}=0.83 V, FF=0.62) and 4.57% (J_{sc}=10.24 mA/cm^2, V_{oc}=0.80 V, FF=0.58) were obtained for devices based on **K2**:PC71BM and **K3**:PC71BM active layers with optimized donor to acceptor weight ratios and processed with a two step annealing treatment. The efficiency of solar cells based on small molecules can be increased considerably by careful engineering and optimization of molecular structure of the blended film morphology.

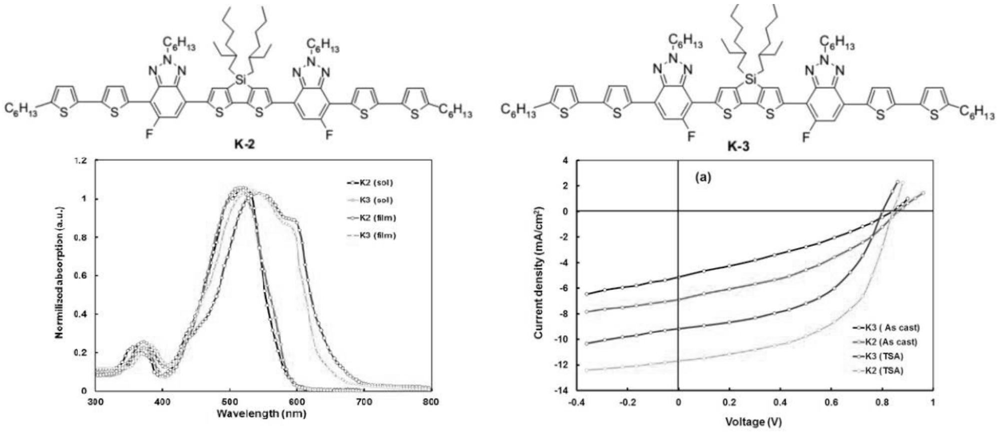

Fig. 1. Structures of K2 and K3, their absorption spectra and *J-V* plots

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P-58

Design and Synthesis of New Ultra-low Bandgap Thiadiazolouinoxaline Based Polymers for Near Infrared Organic Photovoltaic Application

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Two D-A copolymers **F1** and **F2** with fluorene and thiazole units substituted respectively to thiadiazoloquinoxaline (TDQ) unit to enhance the electron-accepting strength of TDQ. The copolymers were synthesized by cross-coupling Stille reaction, and their optical and electrochemical properties were examined revealing that they have ultra low bandgaps, and absorption in the near infrared. These copolymers were employed as donor along with PC71BM as electron acceptor for the fabrication of solution processed bulk heterojunction (BHJ) polymer solar cells. After the optimization of donor to acceptor weight ratio and solvent additive (4% v DIO as solvent additive), the devices with **F1**:$PC_{71}BM$ and **F2**:$PC_{71}BM$ showed power conversion efficiencies (PCEs) of 5.80 (J_{sc}=14.71 mA/cm^2, V_{oc}=0.58 V, FF=0.68) and 3.32 % (J_{sc}=8.92 mA/cm^2, V_{oc}=0.6 V, FF=0.62), respectively. Although **F2** possesses a broader absorption profile as compared to **F1**, the low value of PCE for the **F2** based device has been attributed to the low LUMO offset between **F2** and $PC_{71}BM$ that limited the exciton dissociation. The above results indicate that these copolymers can be utilized for ternary BHJ and tandem solar cells, to achieve the high PCE.

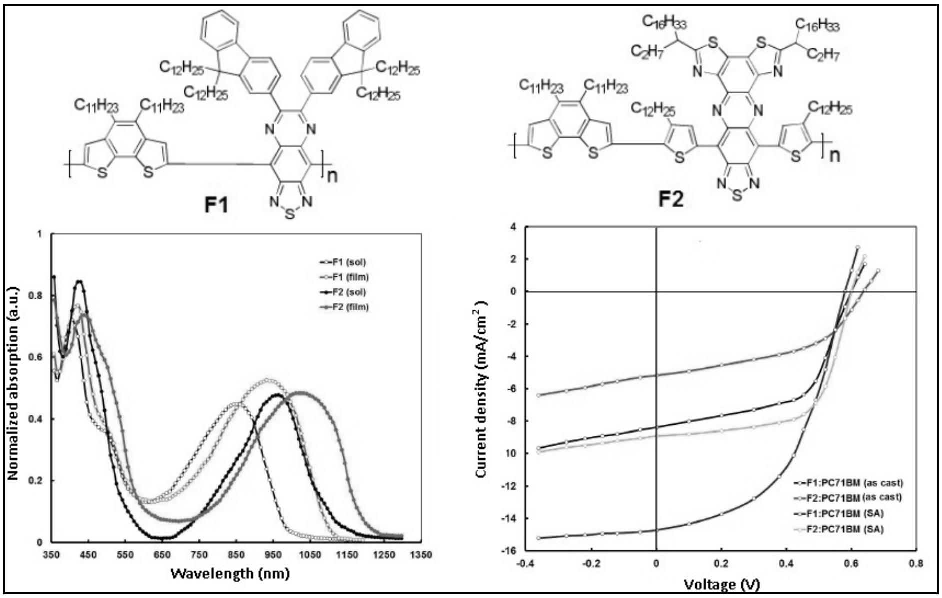

Fig. 1. Structures of the polymers F1 and F2, their absorption spectra and *J-V* plots

M. L. K., D. Yu. G and S. A. K. and thankful to Russian Science Foundation (grant number 14-13-01444).

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P-59

First-principles study of the electronic energy bands and state density of Rock-salt $Zn_{1-x}Sr_xO$ ternary alloys

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Abstract
The structural and electronic properties of $Zn_{1-x}Sr_xO$ ternary alloys in NaCl structures at various Sr concentrations are presented. The calculations are performed using the full potential augmented plane wave (FP-LAPW) method within the density functional theory (DFT) the generalized gradient approximation (GGA) of Perdew et al., Deviation of the lattice constants from Vegard's law and bulk modulus from linear concentration dependence (LCD) were observed for the alloys. The microscopic origins of the gap bowing were explained by using the approach of Zunger and co-workers. In addition, total and partial densities of states and Charge densities were calculated.

Keywords: FP-LAPW, $Zn_{1-x}Sr_xO$, Charge density

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[1] M. Labidi, S. Labidi, F. El Haj Hassan, M. Boudjendlia, R. Bensalem, *Mater. Sci. Semicond. Process* **16** (2013) 1853-1858.

[2] S. Labidi, A. Lakel, M. Labidi and R. Bensalem, *CHIN. PHYS. LETT.* **Vol. 31**, N° 4. (2014) 046104.

P-60

Theoretical investigations of structural, electronic and thermal properties of CdO and ZnO

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First-principles calculations are performed to investigate the structural, electronic and thermal properties of CdO and ZnO in Rocksalt structure using the full-potential linearized augmented plane wave method. In this approach, the generalized gradient approximation (GGA) of Perdew et al. was used for exchange correlation potentials. Moreover, the alternative form of GGA proposed by Engel and Vosko (GGA-EV) and modified Becke-Johnson exchange correlation potential (MBJ) are also used for band structure calculations. Results are given for lattice constant, bulk modulus and electronic properties are in agreement with experimental and theoretical data. The quasi-harmonic Debye model, using a set of total energy versus volume calculations obtained with the FP-LAPW method which is applied to study the thermal and vibrational effects. Temperature effects on the structural parameters, band gap, thermal expansions, heat capacities and Debye temperatures are determined from the non-equilibrium Gibbs functions.

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[1] M. Labidi, S. Labidi, F. El Haj Hassan, M. Boudjendlia, R. Bensalem, *Mater. Sci. Semicond. Process* ***16*** *(2013) 1853-1858*

[2] S. Labidi, A. Lakel, M. Labidi and R. Bensalem, *CHIN. PHYS. LETT.* **Vol. 31**, N 4. (2014) 046104.

P-61

Zn-Ni alloys electrodeposited from alkaline medium bath containing complexing agents

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Keywords: Zn-Ni alloy, Complexing agent, alkaline bath

Abstract.

Ethylenediaminetetraacetic acid, citric acid, and sodium gluconate, were used as complexing agents for the electrodeposition of Zn-Ni alloys, to obtain data concerning their mode of action in order to work out a free alkaline electrolyte containing: 0.16 mol.dm^{-3} ZnO; 3.75 mol.dm^{-3} NaOH; 1.7×10^{-2} mol.dm^{-3}, $NiSO_4.6H_2O$; and 3.4×10^{-2} mol.dm^{-3} of the one of the above complexing agents. The process of electrocrystallization of Zn-Ni alloy onto steel substrate is studied by the electrochemical techniques: cyclic voltammetry, chronopotentiometry, ALSV, and electrochemical impedance spectroscopy. Electrochemical and DRX measurements made it possible to propose an alkaline electrolyte based on citric acid nontoxic and sufficiently stable to obtain better quality Zn-Ni deposits. The polarization behaviour, the microstructure and the stability of the electrolyte were found to depend on complexing agent.

P-62

Liquid – air interface solution growth and structure of large single crystals films of p-quaterphenyl and his novel terminal substituted derivatives

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M.K. Shauhin [2], O.V. Borshchev[2], N.M. Surin[2], S.A. Ponomarenko[2], A. E. Voloshin[1]

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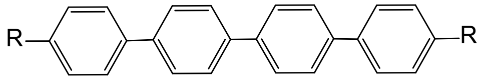
Oligophenyls are known as highly stable and good emitters in the blue region of the spectrum. Single crystalline films of a high quality are essential for light-emitting field-effect devices and lasers fabrication. In this work we report about growth from solutions in the liquid – air interface of large single crystal films[1] of *p*-quaterphenyl (4P) and its novel derivatives with terminal substituents: 4,4'''-di-tert-butyl-1,1':4',1'':4'',1'''-quaterphenyl (tertBu-4P-tertBu) and 4,4'''-bis(trimethylsilyl)-1,1':4',1'':4'',1'''-quaterphenyl (TMS-4P-TMS).



R = -H, $-C(CH_3)_3$, $-Si(CH_3)_3$

The addition of terminal substituents in *p*-quaterphenyl is significantly improves the solubility and interface activity, thereby increasing the growth velocity and providing the formation of large single crystalline films in the interphase boundary. Measurements of the thermal behavior of the investigated substances during heating and melting have been conducted by the differential scanning calorimetry and phase transition points were established. The absorbance and photoluminescence spectra of solutions and crystals have been measured. The obtained crystalline films have been described in detail by the optical, laser confocal and atomic force microscopy. The crystal structure at 295K and 85K has been established by the single crystal X-ray diffraction. The X-ray analysis shows that oligophenyls crystal lattices have the herringbone molecular packing in the crystallographic plane (001) with herringbone angle θ (fig.1.2). A presence of the terminal substituents results in rising the tilt angle χ relatively Z axis (fig.1.3). The growth of thin films along the interface carries out in the crystallographic plane (001) and normally to the interface it occurs layer-by-layer (fig.1.1). Basing on ex situ studies by the confocal microscopy of the substrate surfaces after slow evaporation of solution droplets the resulting data set obtained to identify a mechanism of the thin crystalline films formation at the early stages.

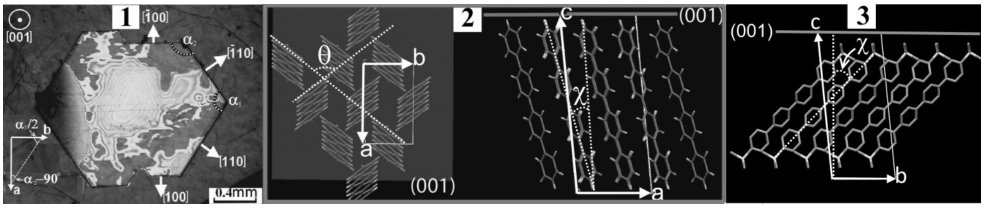


Fig.1. 4P single crystalline film with growth directions (1) and unit cells (001) (left) and (010) projections at 295K (2); (3) TMS-4P-TMS unit cell (100) projection at 295K.

This work is supported by Russian Foundation for Basic Research (project 16-02-00931-a).

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[1] V. A. Postnikov et. al. *Cryst. Growth & Des.* 2014, **14**, 1726−1737.

P-63

The solution processed thin crystal layers formation of organic semiconducting co-oligomers on substrate

M.S. Lyasnikova[1], V.A. Postnikov[1], N.I. Sorokina[1] M.K. Shauhin [2], O.V. Borshchev[2],*
N.M. Surin[2], V.V. Bruevich [3]

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In this work we are reported the investigation results of para-quatrephenyl (4P) and his novel derivatives with terminal substituents “-Si(CH$_3$)$_3$”, “-C(CH$_3$)$_3$” and thiophene-phenylene co-oligomers with terminal substituents “-CH$_3$”, “-Si(CH$_3$)$_3$” and “-C(CH$_3$)$_3$” (Fig.1a) solution substrate thin crystal layers growth. The formation of large single-crystal domain layers on the substrate is an actual scientific and technical problem for the field-effect and light-emitting transistors production technology. It has been applied two growth methods: 1 – growth on horizontal substrate in the slow drying drop of solution (Fig.1b) and 2 – growth on vertical substrate into the volume of slowly drying solution (Fig.1c). The first method allows to obtain the ultra-thin single-crystal layers of thickness from 20 nm to 150 nm and a few millimeters in length during 1-2 hour. The second method application allow to cover the substrate surface of crystal layer with uniform thickness in 1-3 um during the period from several days to several weeks. For the first time the tertBut-PTTP-tertBut large single crystal films has been obtained and solved their crystal structure. It has been identified a number of controllable factors affecting the quality of the formed crystal layers. The nucleation and growth mechanisms is analyzed on the basis of ex-situ obtained empirical data.

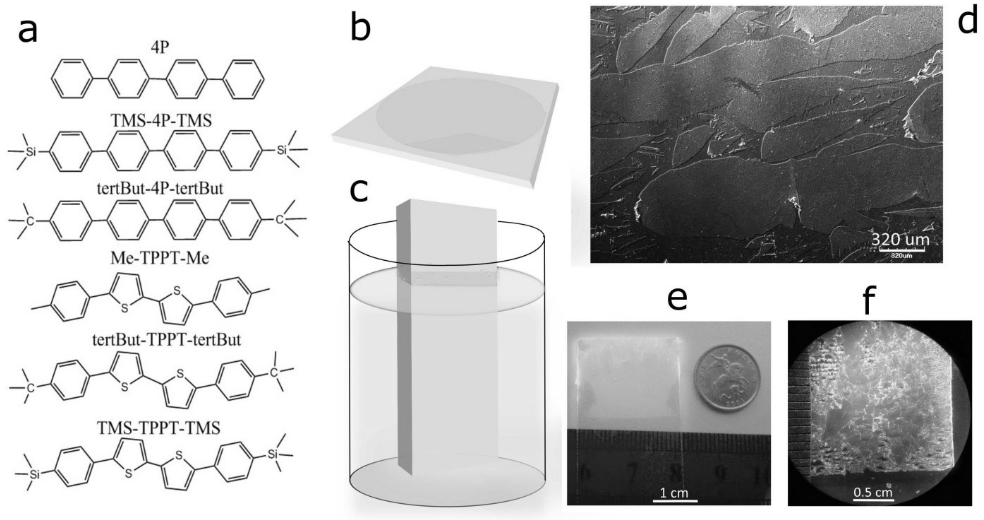

Fig.1. The studied co-oligomers with abbreviation (a); the schematic growth methods: solution drop drying in horizontal substrate (b) and vertical substrate in drying solution (c); the laser confocal micro-image of ultrathin (20-40 nm) single crystal layers of p-quaterphenyl on glass substrate grown at slow solution drop drying (d); the TMS-PTTP-TMS (e) and tertBut-PTTP-tertBut (f) crystal layers on glass substrate under UV.

This work is supported by Russian Foundation for Basic Research (project 16-02-00931-a).

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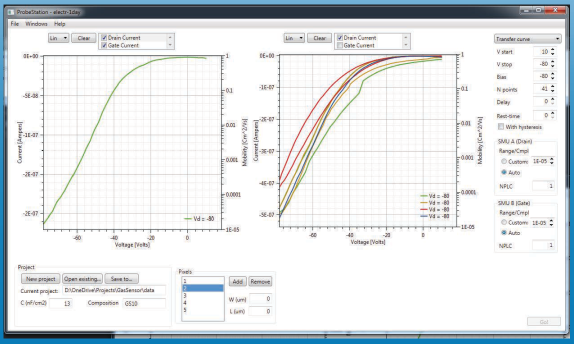

Transfer curve
V start 10
V stop -80
Bias -80
N points 41
Delay 0
Rest-time 0
☐ With hysteresis
SMU A (Drain)
Range/Cmpl
○ Custom: 1E-05
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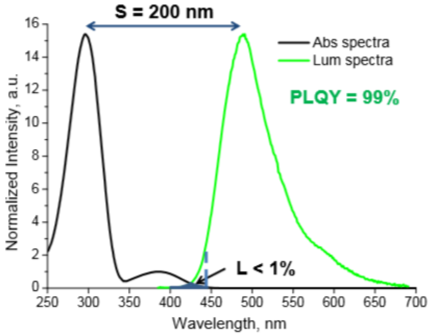

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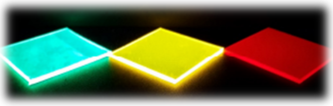

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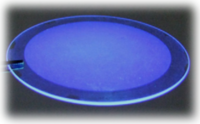

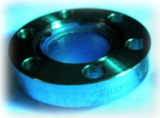

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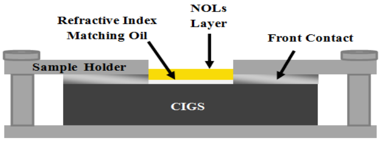

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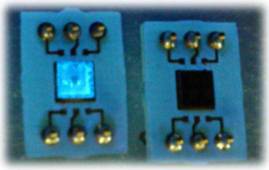

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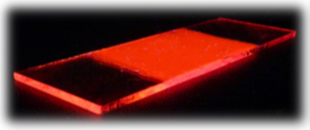

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