



June 4-8, 2017
Saint Petersburg, Russia
Hotel Azimut
<http://www.icoe2017.ru>

13th International Conference on Organic Electronics - 2017 (ICOE-2017)

Book of abstracts



13th INTERNATIONAL CONFERENCE ON ORGANIC ELECTRONICS – 2017 (ICOE-2017)

Organizers

Division of Chemistry and Material Science of Russian Academy of Sciences

Enikolopov Institute of Synthetic Polymer 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)

Federal Agency of Scientific Organizations (FASO RF)

Scientific program

- 1) *Interfaces in organic electronics: understanding and controlling order/disorder and defects*
- 2) *Organic materials challenges in synthesis, design and processing*
- 3) *Organic biosensors for health and environment*
- 4) *Implantable organic electronics and active interfaces to living matter*
- 5) *Hybrid and nanocomposite materials for organic electronics*
- 6) *Organic electronics for energy applications*
- 7) *Organic spintronics*
- 8) *Integration, multifunctionality, flexible and large area technology*
- 9) *Perspectives of organic electronics*



Saint Petersburg, Russia
Hotel Azimut
2017

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Conference program

The 13th International Conference on Organic Electronics – 2017 Time Schedule

	Sunday <i>June 4th</i>	Monday <i>June 5th</i>	Tuesday <i>June 6th</i>	Wednesday <i>June 7th</i>	Thursday <i>June 8th</i>	
9:00		Henning Sirringhaus	Iain McCulloch	Fabio Biscarini	Barbara Stadlober	9:00
		Vitaly Podzorov	Christian Müller	Luisa Torsi	Koen Vandewal	
10:00		Aram Amassian	Christoph Brabec	Annalisa Bonfiglio	Pavel Troshin	10:00
		Coffee-break				
11:00		Oral talks 1	Oral talks 3	Oral talks 5	Oral talks 6	11:00
12:00						12:00
13:00	Registration	Lunch			Closing ceremony	13:00
		Natalie Stingelin	Martin Weis	Hermitage Museum Tour (optional)	Peterhof Excursion (optional)	
14:00		Paul Meredith	Dago de Leeuw			14:00
15:00		Oral talks 2	Oral talks 4			15:00
16:00						16:00
17:00		Coffee-break Poster session 1	Coffee-break Poster session 2	Satellite event (optional)		17:00
18:00	Welcome-party			18:00		
19:00	St. Petersburg Sightseeing Tour	Leisure time	Leisure time	Conference dinner	19:00	
20:00					20:00	
21:00					21:00	
22:00			White-Night Boat Tour (optional)			22:00

Sunday, June 4th

13:00 – 17:30	Registration
17:30 – 19:00	Welcome-party
19:00 – 22:00	Saint Petersburg sightseeing tour

Monday, June 5th

	Chair: <i>Sergey Ponomarenko</i>
9:00 – 9:30	I-1. <i>Henning Sirringhaus</i> . Charge and spin transport physics of organic semiconductors
9:30 – 10:00	I-2. <i>Vitaly Podzorov</i> . Artifact-free determination of the intrinsic charge carrier mobility in high-performance organic field-effect transistors
10:00 – 10:30	I-3. <i>Aram Amassian</i> . Programming the crystallization and microstructure of organic semiconductors
10:30 – 11:00	Coffee-break
	Oral talks 1. Chair: <i>Vitaly Podzorov</i>
11:00 – 11:15	O-1. <i>Tim Leydecker</i> . Polymer blends for precise control of electron and hole transport
11:15 – 11:30	O-2. <i>Kamal Asadi</i> . Graphene ferroelectric field-effect transistors: up-scaling and practicality
11:30 – 11:45	O-3. <i>Thomas Mosciatti</i> . Asymmetric injection in OTFTs via direct SAMs functionalization of electrodes
11:45 – 12:00	O-4. <i>Dario Natali</i> . On the role of metal/semiconductor interfaces and of the density of states in the modeling of organic thin film transistors
12:00 – 12:15	O-5. <i>Muhammad Rizwan Khan Niazi</i> . Two-step nucleation in solution-printed organic semiconductors
12:15 – 12:30	O-6. <i>Thomas Schmaltz</i> . Aligned and region-selective deposition of organic nanowires for thin film transistor applications
12:30 – 12:45	O-7. <i>Rocco Peter Fornari</i> . How many parameters actually affect the mobility of conjugated polymers?
12:45 – 13:00	O-8. <i>Antonio Valletta</i> . Fully printed OTFTs: fabrication and large signal modeling
13:00 – 14:00	Lunch
	Chair: <i>Aram Amassian</i>
14:00 – 14:30	I-4. <i>Natalie Stingelin</i> . Semiconducting: insulating polymer blends – processing, structure and opportunities for the organic electronics field
14:30 – 15:00	I-5. <i>Paul Meredith</i> . Narrow and broadband high detectivity organic semiconductor photodetectors

	Oral talks 2.
15:00 – 15:15	O-9. <i>Laura Basirico.</i> X-Ray imaging with flexible direct organic detectors
15:15 – 15:30	O-10. <i>Le Yang.</i> Efficient triplet exciton fusion in molecularly doped polymer light-emitting diodes
15:30 – 15:45	O-11. <i>Matthew Dyson.</i> Unravelling the effect of side chain environment in conjugated polymers blends
15:45 – 16:00	O-12. <i>Elham Khodabakhshi.</i> Boosting OLED efficiency by blending: spectroscopic identification of reduced charge trapping
16:00 – 16:15	O-13. <i>Elisa Collado-Fregoso.</i> Charge separation and recombination in intermixed and “semi-planar” interfaces: PBTT-T/fullerene blends and solar devices
16:15 – 16:30	O-14. <i>Bernd Ebenhoch.</i> Beyond the Shockley equation: reliable parameter extraction from low-mobility organic solar cells
16:30 – 19:00	Coffee-break Poster session 1 (P-1 – P-50)

Tuesday, June 6th

	Chair: <i>Koen Vandewal</i>
9:00 – 9:30	I-6. <i>Iain McCulloch.</i> Designing high performance organic electronic materials
9:30 – 10:00	I-7. <i>Christian Muller.</i> Interplay between processing and doping of organic semiconductors
10:00 – 10:30	I-8. <i>Christoph Brabec.</i> Physics of non-fullerene acceptors for organic solar cells
10:30 – 11:00	Coffee-break
	Oral talks 3. Chair: <i>Barbara Stadlober</i>
11:00 – 11:15	O-15. <i>Ferdinand Melkonyan.</i> New conjugated connections and substituents for enabling efficient organic materials for photovoltaic and transistor applications
11:15 – 11:30	O-16. <i>Soo Young Park.</i> Designing novel heteroarene molecules for organic electronics: Indolo[3,2-b]indole (IDID) and 1,5-Naphthyridine-2,6-dione (NTD) derivatives
11:30 – 11:45	O-17. <i>Dmitri Godovsky.</i> Conductive polyelectrolytes as a basis for a new generation of electronic devices
11:45 – 12:00	O-18. <i>Yuriy Luponosov.</i> Donor-acceptor molecules with electron-withdrawing phenyldicyanovinyl groups for organic solar cells
12:00 – 12:15	O-19. <i>Maxim Kazantsev.</i> Highly-emissive furan/phenylene co-oligomer single crystals
12:15 – 12:30	O-20. <i>Alexander Shokurov.</i> Structure and complex formation properties of hemicyanine chromoionophore monolayers for sensor applications
12:30 – 12:45	O-21. <i>Francesca Di Maria.</i> Poly(3-hexylthiophene) nanoparticles containing thiophene-S,S-dioxide: tuning of dimensions, optical and redox properties and charge separation under illumination

12:45 – 13:00	O-22. <i>Jens Drechsel.</i> Vacuum Deposition of Perovskite Layers – A New Tool Concept
13:00 – 14:00	Lunch
	Chair: <i>Iain McCulloch</i>
14:00 – 14:30	I-9. <i>Martin Weis.</i> Making polymers conductive by secondary doping
14:30 – 15:00	I-10. <i>Dago de Leeuw.</i> Energy harvesting with PVDF and piezoelectric ceramic-polymer composites
	Oral talks 4.
15:00 – 15:15	O-23. <i>Alexei Komolov.</i> The interface charge transfer and the energy level alignment upon vacuum deposition of the ultra-thin conjugated molecular layers onto solid surfaces
15:15 – 15:30	O-24. <i>Celso de Melo.</i> Flexible self-standing organic supercapacitors of carbon nanotubes/polypyrrole based on eggshell membranes
15:30 – 15:45	O-25. <i>Mari-Cruz Garcia-Gutierrez.</i> Nanopatterning conjugated polymers by laser: influence on electrical properties
15:45 – 16:00	O-26. <i>Dmitry Paraschuk.</i> Self-doping controls luminescence in thiophene-phenylene single crystals
16:00 – 16:15	O-27. <i>Anastasia Glushkova.</i> Thiophene-based single crystal monolayers for organic field-effect devices
16:15 – 16:30	O-28. <i>Oleg Borshchev.</i> Nanostructured organosilicon luminophores for optoelectronics
16:30 – 19:00	Coffee-break Poster session 2 (P-51 – P-126)
19:00 – 22:00	Leisure time
22:00 – 1:00	White-night boat tour (optional)

Wednesday, June 7th

	Chair: <i>Martin Weis</i>
9:00 – 9:30	I-11. <i>Fabio Biscarini.</i> Biorecognition and transduction in ultrasensitive label-free organic biosensors
9:30 – 10:00	I-12. <i>Luisa Torsi.</i> Label-free protein electronic detection with an electrolyte-gated organic field-effect transistor-based immunosensor
10:00 – 10:30	I-13. <i>Annalisa Bonfiglio.</i> Organic Sensing and Biosensing Platforms
10:30 – 11:00	Coffee-break
	Oral talks 5. Chair: <i>Luisa Torsi</i>
11:00 – 11:15	O-29. <i>Beatrice Fraboni.</i> All PEDOT:PSS organic electrochemical transistor for the selective detection of redox-active molecules in biological fluids

11:15 – 11:30	O-30. <i>Laura Ferlauto</i> . Injectable, self-opening, and freestanding retinal prosthesis for fighting blindness
11:30 – 11:45	O-31. <i>Elena Zucchetti</i> . Characterization of organic semiconducting nanoparticles and their <i>in vitro</i> application
11:45 – 12:00	O-32. <i>Andreas Petritz</i> . Single-substrate integrated active-matrix pyro-sensor
12:00 – 12:15	O-33. <i>Alessandro Pezzella</i> . Eumelanin-based electrodes for ITO-free devices in bioelectronics and nanomedicine
12:15 – 12:30	O-34. <i>Andrey Aleshin</i> . Bacterial cellulose modified with conducting and light-emitting polymers for organic biosensors applications
12:30 – 12:45	O-35. <i>Sergey Ponomarenko</i> . Highly sensitive gas sensors based on LS OFETs
12:45 – 13:00	O-36. <i>Alexander Yakimansky</i> . Chromophore-Containing Non-Linearly Optically Active and Light-Emitting Polymers
13:00 – 14:00	Lunch
14:00 – 19:00	Hermitage museum tour (optional)
14:00 – 19:00	Satellite event (optional): Flexible electronics and photovoltaics: from science to markets

Thursday, June 8th

	Chair: <i>Fabio Biscarini</i>
9:00 – 9:30	I-14. <i>Barbara Stadlober</i> . Screen-printing of multifunctional ferroelectric sensors and organic electrochemical transistors on flexible substrates for a multitude of applications such as novel 3D user interfaces, force and proximity sensing surfaces and large-area digital circuits
9:30 – 10:00	I-15. <i>Koen Vandewal</i> . Charge transfer states for organic opto-electronics
10:00 – 10:30	I-16. <i>Pavel Troshin</i> . Novel perovskite and perovskite-inspired materials for solar cells
10:30 – 11:00	Coffee-break
	Oral talks 6. Chair: <i>Dmitry Paraschuk</i>
11:00 – 11:15	O-37. <i>Gitti Frey</i> . Harnessing molecular diffusion in organic solar cell
11:15 – 11:30	O-38. <i>Artem Bakulin</i> . The dynamics of charge separation in organic photovoltaic materials with low electronic band offsets
11:30 – 11:45	O-39. <i>Derya Baran</i> . Fullerene-free organic solar cells exceeding 1V open circuit voltages
11:45 – 12:00	O-40. <i>Stylianos Choulis</i> . Device structure engineering for organic and hybrid photovoltaics
12:00 – 12:15	O-41. <i>Ning Li</i> . Solution-processed organic tandem solar cells: interface design, process optimization and loss analysis

12:15 – 12:30	O-42. <i>Stoichko Dimitrov</i> . Exciton and charge separation dynamics in intermixed polymer:fullerene blends: correlating structural and photophysical length scales
12:30 – 12:45	O-43. <i>Xianjie Liu</i> . Interfacial electronic properties of air-stable molecule-doped polymers and fullerene derivatives for organic photovoltaics
12:45 – 13:00	O-44. <i>Nicola Gasparini</i> . Controlling the recombination in ternary polymer blends: a path towards high efficiency organic photovoltaics
13:00 – 13:30	Closing ceremony
14:00 – 19:00	Peterhof excursion (optional)

Poster session 1

Monday, June 5th, 16:30

Akbulatov, Azat F.	P1	Intrinsic thermal and photochemical stability of hybrid and inorganic lead halide based perovskites
Alim, Cisil	P2	Towards designing new high-mobility polymeric semiconductors: DFT investigation of electronic and optical properties of BTI-based monomers and dimers
Almadhoun, Mahmoud N.	P3	Non-volatile memory devices based on ferroelectric polymer and semiconducting silicon
Anisimov, Daniil S.	P4	Effect of evaporated and laminated gold electrodes on performance of organic single crystal field effect transistors
Baek, Seung Woon	P5	Shellac film as gate insulating layers in organic field-effect transistors
Balakirev, Dmitry O.	P6	Star-shaped donor-acceptor oligomer with p-fluorophenyldicyanovinyl electron-withdrawing groups for organic photovoltaics
Baranov, Denis S.	P7	Synthesis of substituted diaza-analogues of pyrene and perylene
Baranovskii, Sergei D.	P8	Analytical theory for charge carrier recombination in blend organic solar cells
Bof Bufon, Carlos Cesar	P9	Hybrid organic/inorganic interfaces as reversible label-free platform for sensing and biosensing
Botta, Chiara	P10	Stimuli responsive emissive behaviours of organic and organometallic compounds with crystallization induced emission properties
Brackmann, Stefan	P11	Investigation of hybrid organic/inorganic heterostructures in GaN for light emission
Bruevich, Vladimir V.	P12	Vertical cavity laser on thiophene-phenylene co-oligomers
Chekusova, Victoria P.	P13	Metal-containing porphyrins as an active layers for organic field-effect transistors and gas sensors on their base
Cuadrado Santolaria, Alba	P14	Active organic semiconductors based on 10,15-dihydro-5H-diindolo[3,2-a:3',2'-c] carbazole as a centre core for OTFTs
Dashitsyrenova, Dolgor D.	P15	Molecular structure-electrical performance relationship for photochromic materials used in the OFET-based memory devices
Ditte, Kristina R.	P16	Synthesis and photophysical characterization of Y ₃ N@C ₈₀ nitride clusterfullerene's derivatives
Dominskiy, Dmitry I.	P17	Molecular end groups impact on structural and electronic properties of thiophene-phenylene co-oligomer single crystals
Dronov, Mikhail A.	P18	Modeling resistive switching: filamentary model and scaling limits for organic ReRAM
Emelianov, Aleksei V.	P19	The role of carbon lattice functionalization on transport properties in polyaniline molecular channel formed in gap between single-walled carbon nanotubes
Feriancova, Lucia	P20	Effect of electron acceptor groups on molecular properties of potential n-type semiconducting materials
Ferlauto, Laura	P21	Transient electronics for edible neuroprosthetics

Frankenstein, Hadar	P22	Atomic layer deposition of ZnO for top cathode interlayers in organic photovoltaics
Frantseva, Ekaterina S.	P23	Synthesis of furan/phenylene co-oligomers for organic electronics
Frolova, Lyubov A.	P24	Highly efficient all-inorganic planar heterojunction perovskite solar cells produced by thermal co-evaporation of CsI and PbI ₂
Gadirov, Ruslan M.	P25	Inkjet printing of organic semiconductor materials and devices
Galindo, Sergi	P26	Control of structure and morphology of printed thin film organic field-effect transistors
Goryunkov, Alexey A.	P27	Effect of alkyl chain length of double-caged fullerene acceptors on photovoltaic performance
Gudeika, Dalius	P28	Ambipolar 1,8-naphthalimide derivatives exhibiting aggregation enhanced emission phenomenon
Gul'tikov, Nikita V.	P29	Probing of luminescent dopants in single-crystal thiophene-phenylene and furan-phenylene co-oligomers by photothermal deflection spectroscopy
Gurskiy, Stanislav I.	P30	Fluorescent properties of salt built of 3-cyano-4-dicyano-methylene-5-oxo-4,5-dihydro-1H-pyrrole-2-olate anion and 2-aminopyridinium cation
Hietzschold, Sebastian	P31	Nickel oxide as hole contact material in organic electronics: the role of surface chemistry and microstructure
Hofacker, Andreas	P32	Time-dependent recombination orders in organic disordered semiconductors
Hrabal, Michal	P33	Organic electrochemical transistors (OECT) prepared via screen printing technique as a tool for biosensing
Inasaridze, Liana N.	P34	Effect of the substrate and processing conditions on the photochemical, thermal and electrochemical stability of the MAPbI ₃ thin films
Ivanov, Vitaly S.	P35	Iodine-doped carbon nanotube–polyimide composites for microelectronics
Juhasz, Peter	P36	Small- and large-signal analysis of relaxation times in pentacene diode
Keshtov, Mukhamed L.	P37	Synthesis, characterization and photovoltaic properties of new iridium-containing conjugated polymers
Kharlanov, Oleg G.	P38	Description of charge-carrier transport in crystalline organic semiconductors beyond simple hopping or band-transport models
Khotina, Irina A.	P39	Synthesis of hyperbranched oligophenylenes with phenylene ethynylene fragments for optoelectronics
Kiriy, Anton	P40	New highly potent vacuum- and solution-processable [3]-radialene-based molecular p-dopant: synthesis and application
Kleymyuk, Elena A.	P41	Synthesis, theoretical and experimental investigations of new luminescent bithiophenesilane dendrimers
Komissarova, Ekaterina A.	P42	Synthesis and investigation of diaryldiazenes incorporating pyrimidine moiety

Komolov, Alexei S.	P43	Molecular mechanism of reductive dehalogenation by P450 enzymes: possible importance of dissociative electron attachment for biosensor applications
Koskin, Igor P.	P44	Controlling torsional rigidity by introduction of furan moiety into co-oligomers towards highly emissive semiconducting materials
Kotova, Maria S.	P45	Filamentary model of resistive switches in composite structures based on organic dyes and colloidal CdSe nanoplates
Kozlov, Alexey V.	P46	A degradation behavior of the polyquinone-based cathode material for lithium-organic batteries
Krivtsova, Evgenia D.	P47	Linear conjugated oligomers based on 2,1,3-benzothiadiazole as new luminophores for organic photonics
Krupskaya, Yulia	P48	Tuning the charge transfer in organic semiconductor single-crystal interfaces
Kulik, Leonid V.	P49	Structure and spin-dependent recombination of charge-separated state in polymer/fullerene composites
Kwon, Ji Eon	P50	Iptycene-based quinone molecules: multi-electron redox behaviors and application in lithium-ion battery cathodes

Poster session 2

Tuesday, June 6th, 16:30

Leshanskaya, Lidiya I.	P51	Dibenzozindigo: a new nature-inspired semiconductor material for biocompatible organic electronics
Novikov, Artyom V.	P52	Environment friendly aqueous processing of [60]fullerene semiconducting films for organic electronics
Levitsky, Artem	P53	Probing bulk heterojunction morphology of high efficiency organic solar cells by atomic layer deposition
Malov, Vladimir V.	P54	Ambipolar transport in thin layers of new π -conjugated imidazole/carbazole compounds
Mannanov, Artur L.	P55	Stable organic solar cells based on novel highly soluble star-shaped oligomer
Martynov, Ilya V.	P56	The impact of the photoinduced fullerene dimerization vs. generation of stable free radicals on the outdoor operation stability of organic solar cells
Maslennikov, Dmitry R.	P57	Surface-enhanced raman spectroscopy of thiophene-phenylene co-oligomer semiconducting monolayer
Micjan, Michal	P58	Influence of electrode material on contact resistance of organic field-effect transistors
Moshkalev, Stanislav A.	P59	Thin films based on multilayer graphene nanobelts and quantum dots deposited by modified Langmuir-Blodgett technique
Mróz, Wojciech	P60	Push-coating: a low-cost and green fabrication approach to polymer electronic devices
Mróz, Wojciech	P61	Water/alcohol soluble conjugated polymers as electron-injecting layers for OLED technology
Müller, Lars	P62	Controlled drift of small molecule dopants in organic semiconductors
Mumyatov, Alexander V.	P63	Theoretical and experimental study of the capacity fading in lithium-poly(naphthalene diimide) batteries

Nevostruev, Danil A.	P64	Non-fullerene tetraazaperylene-based electron acceptors for organic photovoltaics: EPR measurements
Novota, Miroslav	P65	Characterization of naphthalene derivatives with different alkyl side chains
Obrezkov, Filipp A.	P66	Effect of substituents in photochromic materials of di(hetaryl) ethene series on electrical characteristics of memory devices based on organic field-effect transistors
Obuchovsky, Stas	P67	Probing the amorphous domains in P3HT/Fullerene blends
Odod, Aleksey V.	P68	Photo- and electroluminescence of metal-organic complexes with zinc and beryllium
Pakhomov, Georgy L.	P69	Characterization of organic-based devices by ToF-SIMS depth profiling
Platonova, Elena O.	P70	Red light-emitting polynorbornenes with cyclometaled iridium(III) complexes, carbazole and organosilicon groups in side chains
Polinskaya, Marina S.	P71	Novel organosilicon derivatives of [1]benzothieno[3,2-b][1]-benzothiophene: synthesis and semiconductor properties
Postnikov, Valeriy A.	P72	Crystals of organic conjugated rod-like co-oligomers: structure and peculiarities of growth from solutions
Promarak, Vinich	P73	A Significant improvement of dye-sensitized solar cell (DSSC) performance by donor substitutions on the π -linker of D- π -A organic dye
Raychev, Deyan	P74	A step-by-step theoretical study of monomers for all-conjugated block-copolymers
Ryoo, Chi Hyun	P75	Indolo[3,2-b]indole as a new electron donor for efficient thermally activated delayed fluorescence (TADF) emitters in organic light-emitting diodes (OLEDs)
Saunina, Anna Yu.	P76	Analytic modelling of field dependence of charge mobility in organic materials with correlated disorder
Selektor, Sofiya L.	P77	Nonradiative energy transfer in multilayer Langmuir-Blodgett films based on fluorophores of different chemical structure
Selivanova, Daria G.	P78	Synthesis, optical and electrochemical study of new bipolar heterocyclic systems, including 1,2,4-oxadiazole moiety
Shamieh, Basel	P79	Spontaneously generated interlayers in direct and inverted OPVs with silver and gold contacts
Sharifi Dehsari, Hamed	P80	Toward solution processed magnetic nanoparticles for non-volatile memory applications
Sharifi Dehsari, Hamed	P81	Ambient processing of P(VDF-TrFE) ferroelectric thin-films for application in non-volatile memory devices
Shcherban, Valentina V.	P82	Planar thin-film memristors based on polyaniline and polyethylene oxide
Shklyaeva, Elena V.	P83	Some new nitrogen-containing heterocyclic systems, including ferrocene moiety
Sizov, Alexey S.	P84	Sorption and desorption processes of toxic gases and water vapour in monolayer Langmuir-Schaefer organic field-effect transistors

Skorotetsky, Maxim S.	P85	Novel reactive nanostructured organosilicon luminophores and scintillators on their basis
Solodukhin, Aleksandr N.	P86	Novel donor-acceptor oligomers having different architecture based on triphenylamine for organic photovoltaics
Sosorev, Andrey Yu.	P87	Unravelling the mechanism of outstanding electron mobility in F ₂ -TCNQ single crystals
Susarova, Diana K.	P88	Ammonia gas sensors based on fluorinated naphthalenediimide semiconductor films
Talalaev, Philip S.	P89	BODIPY as a versatile material for memory elements and photodetectors
Toropynina, Victoria Y.	P90	Unsymmetrical donor-acceptor oligomers based on triphenylamine: synthesis and properties
Trukhanov, Vasily A.	P91	Effect of space charge limited current under the source and drain contacts on the performance of organic field-effect transistors
Trukhanov, Vasily A.	P92	Numerical modeling of power conversion efficiency in organic light-emitting transistors
Trul, Askold	P93	Influence of a chemical structure of organosilicon BTBT derivatives on their electrical performance in ultrathin OFETs prepared by different techniques
Uvarov, Mikhail N.	P94	Novel anthrathiophene-based small molecules as donor material for organic photovoltaics: Synthesis and light-induced EPR study
Velasco, Dolores	P95	Influence of the crystallinity of the organic thin film layer in OTFTs
Vinokur, Jane	P96	On the dynamics of additive migration to form cathodic interlayers in OPVs
Weiter, Martin	P97	Diketopyrrolopyrrole based OTFTs with high performance
Yamilova, Olga R.	P98	Towards understanding the photochemical degradation pathways of conjugated polymers under anoxic conditions
Yoshida, Yuji	P99	Various aspects of organic photovoltaics: the low illuminance and polarization
Zhang, Qiaoming M.	P100	High performing solution-coated electrolyte-gated organic field-effect transistors
Viola, Fabrizio Antonio	P101	Ultrathin, flexible multimodal sensor based on organic field effect transistor for tactile sensing applications
Agumba, John O.	P102	Tuning the optical absorption of P3HT single crystals for opto-electronic applications
Bakiev, Artur N.	P103	Synthesis of new conjugated systems composed of 2,5-di(2-thienyl)pyrrole moieties: investigation of optical and electrochemical properties
Bortolotti, Carlo Augusto	P104	EGOFETs with immobilized peptide aptamers as biosensors for ultra-sensitive detection of protein biomarkers in complex fluids
Fisyuk, Alexander S.	P105	Structures-electronic properties relationships for the family of five-membered π -conjugated heterocyclic donor-acceptor-donor oligomers
Freidzon, Alexandra	P106	Theoretical prediction of operational stability of potential OLED host molecules by multireference quantum chemistry

Haddad, Clara	P107	Introduction of Lambert-function based method for OTFT modelling and application to low temperature measurements
Huang, Hui	P108	The nonbonding conformational locks for constructing highly planar π -conjugated systems
Ismail, Moneim	P109	Some complex bismuth-based halides as lead-free materials for "perovskite" solar cells
Kaiser, Christina	P110	Substituted bithiopyranylidenes and their CT complexes with C60 for organic near-infrared detectors
Kalyani, Neeti	P111	Molecular FET based on recombinant azurin protein with enhanced switching behavior
Kochervinskii, Valentin V.	P112	Influence of electrode materials on highfield polarization and conductivity of the ferroelectric copolymers of vinylidene fluoride and tetrafluoroethylene
Kostyuchenko, Anastasia	P113	Synthese of new 5,5'-bis(3-decyl-[2,2'-bithiophen]-5-yl)-2,2':5,2'':5'',2'''-quater(1,3,4-thiadiazole)
Li, Shuo	P114	Improving performance of transistor memory by tuning occurrence charge transport on pentacene interaction
Lmimouni, Kamal	P115	Improving performance of nano-floating memory by tuning occurrence charge transport on pentacene interaction
Majhi, Koushik	P116	Photophysical studies of inclusion complex formation of 3-aminophenol with β -cyclodextrin
Nikitenko, Vladimir R.	P117	Analytic model of mobility and field-stimulated diffusion coefficient in disordered organic semiconductors
de Oliveira, Helinando P.	P118	Development of polypyrrole-based organic composites in electrospun fibers applied in bacterial removal from surfaces
Peng, Yingquan	P119	Near-infrared photo detectors based on organic semiconductors
Peng, Yingquan	P120	Broadband photodetectors based on organic semiconductor
Raisys, Steponas	P121	Enhanced efficiency of light upconversion <i>via</i> emitter structural modification
Ramakrishna, Jagarapu	P122	Facile synthesis, fluorescence and OFET properties of larger fluorenes
Shcherbina, Maxim A.	P123	Modern approaches to the studies of thin films: X-ray reflectometry and grazing incidence scattering
Shcherbina, Maxim A.	P124	Comparative analysis of the structure and phase behavior of carbosilane dendrimers based on α,α' -dialkylquatrothiophene
Speller, Emily M.	P125	Photo-oxidation of electron acceptors and their blends
Shushin, Anatoly I.	P126	Manifestation of T-exciton migration in the kinetics of singlet fission in organic semiconductors
Viani, Lucas	P127	Resonant energy transport in dye-filled monolithic crystals of zeolite L: Modeling of inhomogeneity

Satellite event

Flexible electronics and photovoltaics: from science to markets

Flexible electronics and photovoltaics nowadays step into technological implementation and commercial realization phases. The emerging market of highly integrated flexible electronic devices requires seamless conversion of scientific developments into real products for end-users.

On June, 7th ICOE-2017 participants are invited to attend a Satellite event “Flexible electronics and photovoltaics: from science to markets” organized by ITMO University (Saint-Petersburg), Technospark Nanotech center (Moscow, Troitsk) and North-West Nanotech center (Saint-Petersburg).

Satellite event program:

14:00 – **Shuttle bus transfer from Azimut hotel to ITMO University (Lomonosova str., 9)**

14:30 – **Welcome coffee**

Tour for Organic Electronics and Photovoltaics Laboratory of ITMO “Flexible electronics and photovoltaics: from science to markets” session.

Invited speakers are top researchers and business people in the field of flexible electronics and photovoltaics. The following presentations are scheduled on June, 7th:

1. *Ronn Andriessen*, Program Manager, Solliance, TNO/Holst Centre, “Towards Roll-to-Roll upscaled high efficient Perovskite based flexible solar cells and modules”.
2. *Cedric Rolin*, Senior researcher, Imec (Belgium) “Deposition of Organic Semiconductors: a path to effective devices”.
3. *Mike Banach*, Technical director FlexEnable (UK), “OTFT Technology: Enabling Transformational New Applications”.
4. *Denis Kovalevich*, CEO, Technospark Nanotech centre (Russia), “Venture business model for global industry of flexible electronics: partnerships and infrastructure”.
5. *Viktoria Zheltova*, Director Organic Electronics and Photovoltaics Laboratory at IFMO University (Russia), “Organic Electronics and Photovoltaics Laboratory in the framework of technological transfer”.
6. *Boris Galkin*, Executive director TEN FLECS (Russia), “Bridging the gap between R&D and mass manufacturing: prototyping and small scale manufacturing facility for thin-film electronics”.

Coffee break

Official opening ceremony of Organic Electronics and Photovoltaics Laboratory with ITMO University, dean Vladimir Vasiliev.

Satellite day organizers announcements.

Award ceremony for the best projects.

18:00 – 18:30 – **Shuttle bus transfer to Azimut hotel**

Invited lectures

Charge and spin transport physics of organic semiconductors

H. Sirringhaus¹

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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 device operation, good operational stability and other functionalities such as efficient electroluminescence, sensing or memory functions for a variety of applications. We are interested in understanding the spin and charge transport physics of these materials and the relationship between molecular structure, microstructure and spin and charge diffusion. Organic semiconductors may enable realisation of long spin relaxation times and long spin diffusion lengths due to the weak spin-orbit coupling but it is difficult to achieve efficient spin injection by conventional electrical injection from spin-polarised ferromagnetic metals due to impedance mismatch. We have developed a method for efficient spin injection into these highly resistive materials using the technique of spin pumping using ferromagnetic resonance induced at the interface between ferromagnetic metals or insulators and organic semiconductors. In this talk I will give an overview over the physics of molecular and polymer semiconductors and discuss their relevance for applications in large-area electronics, spintronics and quantum information.

Artifact-free determination of the intrinsic charge carrier mobility in high-performance organic field-effect transistors

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Organic field-effect transistors (OFETs) are the primary building blocks of organic electronics, the field aiming at developing inexpensive, flexible circuits for optoelectronics and power harvesting applications. Studies of OFETs are necessary for understanding the transport properties of organic semiconductors, including their charge carrier mobility. However, the literature is plagued by reports with erroneous mobility values obtained in less than optimal devices. In such cases, mobility is frequently overestimated either due to incorrectly functioning OFETs or wrong mobility extraction procedures applied to experimental data. In addition, there exist several prominent device and measurement related artifacts that are frequently ignored by the authors, thus leading to wrong mobility values as well.

In order to better understand the *intrinsic* transport properties of organic semiconductors, it is firstly necessary to study devices based on high-purity molecular single crystals, in which the intrinsic properties of organic semiconductors can be revealed without parasitic effects of disorder¹. Secondly, the device and measurement related artifacts, as well as poor practices in mobility extraction from OFET data must be understood and avoided (for a discussion of some of these issues see Fall MRS-2012 tutorial²). Finally, in order to obtain solid data on the intrinsic carrier mobility, it is necessary to perform a minimum set of control experiments, including measurements of OFETs both in the linear and saturation regime, evaluation of the contact resistance (by a gated 4-probe or other techniques), as well as measurements of the Hall effect^{3,4,5} and temperature dependence of mobility $\mu(T)$ (the latter two measurements are necessary, if a high mobility is claimed).

This talk will overview some of the main achievements and recent progress in single-crystal OFET devices, describe the most typical artifacts in mobility determination in OFETs and how to avoid them, and it will finally present a “check list” of the required minimum set of measurement that must be performed by researchers working on OFETs, especially in the cases when a high mobility ($> 1 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$) is claimed.

¹ V. Podzorov, *themed issue of MRS Bulletin*: “Organic Single Crystals: Addressing fundamentals of organic electronics” introductory paper, *MRS Bulletin* 2013, **38**, 15-24.

² Tutorial slides are downloadable at <http://www.physics.rutgers.edu/~podzorov/index.php>

³ V. Podzorov *et al.*, “Hall effect in the accumulation layers on the surface of organic semiconductors”, *Phys. Rev. Lett.* 2005, **95**, 226601.

⁴ Y. Chen, H. T. Yi, V. Podzorov, “High-Resolution *ac* Measurements of the Hall Effect in Organic Field-Effect Transistors”, *Phys. Rev. Applied* 2016, **5**, 034008.

⁵ H. T. Yi, Y. N. Gartstein, V. Podzorov, “Charge carrier coherence and Hall effect in organic semiconductors”, *Sci. Reports* 2016, **6**, 23650, DOI: 10.1038/srep23650.

Programming the Crystallization and Microstructure of Organic Semiconductors

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The functional properties and performance of polycrystalline semiconductors are determined by the structure, geometry and spatial distribution of their multitude of crystals. The high anisotropy of molecular building blocks and the associated anisotropic transport properties in organic crystals, make the spatial arrangement and orientation of crystalline domains in polycrystalline organic semiconductors particularly crucial to achieving consistently excellent transport properties uniformly in large area printed electronic applications. A key challenge of polycrystalline thin film processing is that crystallization is seeded through stochastic and incoherent nucleation events, limiting the ability to control or pattern the microstructure, texture, and functional properties of polycrystalline materials as needed, for instance, for electronic circuit or display applications. Contact induced nucleation and directional crystallization through knife coating and related methods have been proposed to mediate polycrystalline microstructure, but these methods suffer other limitations and do not provide total control over the microstructure of polycrystalline films. We present a universal approach that can program the microstructure of materials through the coherent seeding of otherwise stochastic homogeneous nucleation events.¹ The method relies on creating topographic variations to seed homogeneous nucleation events which grow at designated locations while nucleation is inhibited elsewhere. Each seed can thus produce a coherent growth front of crystallization with a geometry designated by the shape and arrangement of seeds. Periodic and aperiodic crystalline arrays of functional materials, such as semiconductors, can thus be created on demand and with unprecedented sophistication and ease by patterning the location and shape of the seeds. This approach is used to demonstrate printed arrays of organic thin-film transistors with remarkable performance and reproducibility owing to their demonstrated spatial control over the microstructure of polycrystalline materials.

This work was supported by the King Abdullah University of Science and Technology (KAUST).

¹ L. Yu, M. R. Niazi, G. O. N. Ndjawa, R. Li, A. R. Kirmani, R. Munir, A. H. Balawi, F. Laquai, A. Amassian *Science Advances* 2017, **3** (in press).

Semiconducting:insulating polymer blends – Processing, structure and opportunities for the organic electronics field

*N. Stingelin*¹

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Polymeric semiconductors promise the possibility to fabricate electronic devices by a variety of low cost printing techniques. They also offer an unprecedented versatility to tune their optoelectronic features via synthetic means. However, in order to enable the next generation plastic electronics devices, such as logic circuits, solar modules or bioelectronic sensors, an additional property matrix in terms of suitable solution rheology for printing purposes, mechanical flexibility for rollable applications and environmental stability needs to be fulfilled as well. Here, the design of multicomponent systems, often via use of additives and isolating polymers as a second species, will be discussed and different strategies presented that permit control of solution parameters, film robustness, and overall device stability. As an example we will discuss polymer transistors where in addition to fast switching and high charge mobilities, other device parameters are often of critical importance for real applications. We demonstrate, for instance, that a low operation voltage, low OFF-current and a low gate leakage can be realised via blending while also keeping the threshold voltage low and drastically more stable. Possible reasons for this beneficial effect will be discussed and extensions to other materials systems and devices discussed.

Narrow and Broadband High Detectivity Organic Semiconductor Photodetectors

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The mainstay of traditional and current commercial photodetectors for the UV-visible-NIR region are based upon inorganic semiconductors that either operate in a photovoltaic or photoconductive mode¹. A broadband response such as that provided by silicon photodiodes yield spectrally flat detectivities of order 10^{13} Jones, and input optical filtering (red, green and blue) is used to create narrow spectral responses for imaging applications. In the past decade a host of new photodetector materials have emerged which can be simply and cheaply processed and deliver comparable detectivities, linearities and improved (lower) power consumption¹. In particular, organic semiconductors in photo-field-effect-transistor, photodiode and photoconductive gain modes are showing significant promise in both broadband and spectrally selective applications^{1,2}.

In my talk I will discuss how organic semiconductors can be designed and tuned to deliver broad-and-narrow-band specific detectivities of order 10^{12} Jones and linear dynamic ranges of ~ 200 dB. With appropriate charge transport layers, extremely low dark noise currents can be achieved of < 0.1 nA³. I will also discuss the concept of charge collection narrowing whereby seemingly broad spectral response organic semiconductor acceptor-donor blends can be engineered to deliver < 100 nm FWHM narrowband responses without the need for input optical filtering⁴.

¹ F.P. García de Arquer, A. Armin, P. Meredith & E.H. Sargent, *Nature Reviews Materials* 2017, **2**, 16100.

² R. Jansen van-Vuuren, A. Armin, A.K. Pandey, P.L Burn & P. Meredith, *Advanced Materials* 2016, **28(24)**, 4766-4802.

³ A. Armin, M. Hamsch, I.K. Kim, P.L. Burn, P. Meredith & E.B. Namdas, *Laser and Photonics Reviews* 2014, **8(6)**, 924-932.

⁴ A. Armin, R. D. Jansen-van Vuuren, N. Kopidakis P. L. Burn & P. Meredith, *Nature Communications* 2015, **6**, 6343.

Designing high performance organic electronic materials

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Understanding the impact of both the organic semiconductor design and processing conditions, on both molecular conformation and thin film microstructure is essential in achieving the required optical and electrical properties of organic electronic devices. For example, the charge carrier mobility in an organic field effect transistor can be significantly increased through appropriate optimization of the semiconductor molecular conformation and self-assembly. These aspects will be explored with an indacenodithiophene polymer as a case study. Organic solar cell efficiencies are currently increasing rapidly based on organic bulk heterojunction devices fabricated from solution. During this period, the structural diversity of semiconducting donor polymers for solar cells has increased dramatically, enabling accelerated development of bulk heterojunction (BHJ) organic solar cells based on polymer donor materials and molecular fullerene derivatives. However both the fullerenes, and the low bandgap polymers typically suffer from low absorption coefficients due to weak oscillator strength. Our approach has been to use P3HT as a p-type hole acceptor, and design highly absorbing, low-bandgap n-type small molecules to replace fullerenes. These fullerene acceptors not only have weak absorption, but also poor tunability of absorption over the longer wavelengths of the solar spectrum; morphological instability in thin film blends over time; high synthetic costs and limited scope for synthetic control over electronic and structural properties. For these reasons, we have developed new, synthetically simple electron acceptor materials, based on rhodanine end groups, which have much larger absorption coefficients than fullerenes, coupled with high lying LUMO energy levels, to maximize cell voltages. In BHJ devices with P3HT donor polymer, the rhodanine molecules were demonstrated to outperform all fullerenes.

Interplay between Processing and Doping of Organic Semiconductors

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Molecular doping of organic semiconductors is an important tool for the optimization of electronic devices ranging from field-effect transistors to solar cells and thermoelectric generators. In this talk the interplay between processing and the solid-state nanostructure of molecularly-doped conjugated polymers will be discussed, and relevant structure-property relationships will be established. Design criteria that permit to mitigate the often encountered poor compatibility of molecular dopants and organic semiconductors will be introduced. As an example, co-processing of a polythiophene and common molecular dopants will be discussed, resulting in thermally stable films with a high electrical conductivity of 100 S/cm. Finally, the use of insulating matrix polymers will be revisited, which can be used to adjust the rheological and mechanical properties of electrically conducting plastics.

Physics of non-fullerene acceptors for organic solar cells

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Non fullerene acceptors impressed the community by their rapid development. After a long and difficult early stage development, the non fullerene acceptors (NFA) saw a surprising breakthrough during the last years. Efficiencies of over 10 %, record lifetimes of several 1000s of hours under illumination without degradation and high performance printed modules were already demonstrated with the last two years. The potential low costs of these acceptors round up their attractive profile for applications. Even more fascinating is the complex device and photo-physics of these non-fullerene acceptors, which is found to be dramatically different to the one of fullerenes. An outstanding low mobility in equilibrium is balanced by unusual high carrier lifetimes, overall resulting in a distinct device operation. The nature of the long carrier lifetime in parallel to the ultrafast generation rate of less than 7 fs is currently not fully understood. This presentation will introduce into the physics of NFA composites and devices and then tries to link the photo-physical properties of NFAs to their molecular design.

Making Polymers Conductive by Secondary Doping

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Organic electronics have potential applications in optoelectronic devices that are usually represented by sandwich structures and require application of a transparent conductive layer for one of the electrodes. Common transparent conductive oxides (TCOs) such as indium tin oxide and doped zinc oxide (ZnO) suffer from high-cost deposition methods and low flexibility. The material research represented by Heeger and his coworkers in the 1970s proposed polymers with π -conjugated bonds as a promising candidate for organic conductive materials and an alternative to TCO. Although various polymers such as polyacetylene, polypyrrole, polythiophene, and polyphenylene have been studied, one of the most popular materials for conductive layer applications is still poly(3,4-ethylenedioxythiophene):poly(4-styrenesulfonate) (PEDOT:PSS). One of the significant limitations was insufficient electrical conductivity ranging from 10^{-6} to 10^{-1} S/cm. As a result, many research groups made a great effort to improve the conductivity by material doping. It has been reported that various polyols, amides, sulfoxides, anionic surfactant, and salts increase the conductivity by two to three orders of magnitude if the dopant is added to the solvent. Furthermore, it has been reported that the post-treatment by immersion of the solid film into the dopant is also capable to improve the conductivity greatly.

Here we demonstrate the microscopic effect of the secondary doping. Although the secondary dopant is not included into the film structure, it causes the enhancement of electrical conductivity as well as the change of the microscopic structure represented by the phase separation of PEDOT and PSS. As a result, the charge transport due to variable range hopping (VRH) is changing the dimensionality from 1D to 3D. The time dependence of the conductivity enhancement is also discussed for the case of the post-treatment technique where the great increase of the conductivity appears in very first seconds.

This work was supported by the Slovak Research and Development Agency (grants APVV-14-0739 and APVV-14-0740).

Energy harvesting with PVDF and piezoelectric ceramic-polymer composites

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The ability to deliver sustainable power to a wireless sensor network is attractive as it eliminates the time and cost of replacing batteries. This holds especially for networks that are either inhospitable or difficult to reach, such as structure-embedded microsystems and medical implants. For small electronic devices the most attractive energy source is that of mechanical vibrations. There are various methods to harvest the mechanical energy but the most widely investigated effect is piezoelectricity. The direct effect is used, where application of a mechanical stress generates an output voltage. The power density for piezoelectric transduction exceeds that for electromagnetic and electrostatic generators below a volume of about 1 cm³.

The efficiency is strongly frequency dependent as the piezoelectric material generates maximum power at resonance frequency. For vibrations of 1 kHz or higher, the obvious choice therefore is piezoelectric ceramics. However, most vibration sources, such as human motion, kitchen appliances and car engines, generate much lower frequencies. For those high strain applications, mechanically flexible materials with a small Young's modulus are required, such as piezoelectric polymers or ceramic-polymer composites.

In this presentation we will analyse the performance of flexible piezoelectric materials for energy harvesters. We will show how the piezoelectric charge coefficient of the homopolymer polyvinylidene fluoride (PVDF) and its random copolymers with trifluoroethylene (P(VDF-TrFE)) can be improved. On the other hand flexible piezoelectric films can be made by dispersing inorganic ceramic particles into a polymeric matrix. However, the piezoelectric properties typically suffer by the limited connectivity between the electro-ceramic particles. We will show that their performance can be dramatically improved by aligning the particles using dielectrophoresis.

Biorecognition and transduction in ultrasensitive label-free organic biosensors.

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Biorecognition is a central phenomenon in all biological processes, including technological and health applications. I will discuss how Electrolyte Gated Organic Field Effect Transistors (EGOFETs) can be used to study and quantitatively extract the thermodynamics of biomolecular recognition between a recognition moiety (an antibody or a peptide aptamer) at an active interface and a relevant target protein. Different cytokines will be shown as relevant biomarkers for inflammatory pathologies. The EGOFET biosensor exhibits a non-intuitive super-exponential response at concentrations below 1 nM with a level of detection below 100 pM with antibodies and down to 300 fM with peptide aptamers. The sensitivity of the device depends on the analyte concentration, reaching a maximum below 1 nM and when the EGOFET is operated in the sub-threshold regime. Conversely, at larger concentrations the response is linear. The sensitivity and the dynamic sensing range are modulated by the gate voltage. This allows us to infer the direct correlation between the sensitivity and the density of states (*DOS*) of the organic semiconductor, i.e. the observed super-exponential trend mirrors the energy-dependence of the tail of the *DOS* of the HOMO level. From the voltage-dependent response, we extract the affinity binding constant, the binding free energy and the changes of the surface charge and capacitance. Finally, we demonstrate the possibility of using EGOFET sensor in human fluids and attempt a comparison with ELISA, as a relevant example of application at point-of-care.

Label-free protein electronic detection with an electrolyte-gated organic field-effect transistor-based immunosensor

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Organic bio-electronics represents one of the most exciting directions in printable electronics, promising to deliver new technologies for healthcare and human well-being. Among the others, organic field-effect transistors have been proven to work as highly performing sensors¹. Selectivity is achieved by integrating a layer of functional biological recognition elements, directly coupled with an electronic interface. The devices were shown to reach detection limits down to the picomolar (10^{-12} M) range^{2,3} with highly repeatable responses (within few percentage of standard deviation) even for hundreds of reiterated measurements.

In this lecture recent developments in the field of organic and printable electronics implemented to probe biological interfaces will be discussed highlighting the importance of the interplay among disciplines such as organic electronics, analytical chemistry and biochemistry to reach a comprehensive understanding of the underpinning phenomena. It will also be shown that applications can lead to label-free electronic biosensors with unprecedented detection limits and selectivity. Notably, the extremely good sensing performance level can be rationalized by quantifying electrostatic and capacitance contributions characterizing the surface confined biological recognition elements interacting with their affinity ligands. Examples of the detection of clinical relevant biomarkers will be provided too.

¹ Manoli, K.; Magliulo, M.; Mulla, M.Y.; Singh, M.; Sabbatini, L.; Palazzo, G.; Torsi L. *Angewandte Chemie International Edition* 2015, **54**, 2-17.

² Macchia, E.; Alberga, D.; Manoli, K.; Mangiatordi, G.F.; Magliulo, M.; Palazzo, G.; Giordano, F.; Lattanzi, G.; Torsi, L. *Scientific Reports* 2016, **6**:28085.

³ Mulla, M.Y.; Tuccori, E.; Magliulo, M.; Lattanzi, G.; Palazzo, G.; Persaud, K.; Torsi, L. *Nature Communications* 2015 **6**:6010.

Organic Sensing and Biosensing Platforms

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The introduction in the early 70s of the Ion Sensitive Field Effect Transistor (ISFET) represented a real turning point in several fields since it allowed the realization of compact, label-free, and versatile sensors and biosensors based on the concept of transistor meant as a charge sensor. Despite their great potentiality, ISFET-like devices generally suffer from an intrinsic limitation in sensitivity, the so-called Nernst limit. Moreover, the high costs, the restricted range of employable materials associated to the silicon technology, and the need for a reference electrode, have reduced the applicability of such devices in the bio-sensing field, in particular in *in vivo* applications. We have developed a reference-less sensor based on an organic semiconductor device, called Organic Charge-Modulated Field-Effect Transistor (OCMFET), that thanks to its peculiar transduction principle and structure, offer the possibility to modulate its sensitivity by acting on geometry-related parameters of the device itself. The proposed approach has been applied to several sensing tasks as, for instance, pH, DNA detection, monitoring of cell electrical activity, etc., thus giving rise to a new family of highly sensitive, reference-less, and low-cost devices for a wide range of bio-sensing applications.

Screen-printing of multifunctional ferroelectric sensors and organic electrochemical transistors on flexible substrates for a multitude of applications such as novel 3D user interfaces, force and proximity sensing surfaces and large-area digital circuits

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²The Fraunhofer Institute for Silicate Research

Screen printing is one of the most common techniques used in printed electronics for the fabrication of large-area flexible components and multifunctional devices. It is highly tolerant to the type and form factor of substrates, the rheology of ink materials, provides sufficient alignment accuracy for multilayer printing and can be done in a sheet-to-sheet or roll-to-roll scheme.

Here we present the usage of this well-known method for the large-area fabrication of two kinds of flexible devices: ferroelectric sensors and organic electrochemical transistors (OECT) and combinations thereof. The sensors are based on the ferroelectric material PVDF:TrFE which supports both – the pyro- and the piezoelectric effect useable for sensing pressure, impact forces and bending interaction on large, flexible surfaces and for detecting IR radiation and the proximity of human beings. The sensors have a sandwich structure of four layers that are printed onto any flexible and bendable substrate (e. g. plastic foils, paper, and textiles) over large areas (up to A3) and response accurately, fast and reproducibly to pressure and temperature changes over large dynamic ranges. By optimizing the design, the printing and annealing process as well as the poling conditions and the source material functional sensors with a soft yield of more than 98% with less than $\pm 5\%$ deviation in the remnant polarization were demonstrated. It is also interesting to note that extended aging tests under definite climate and shock conditions revealed more than 98% preservation of the remnant polarization for high molecular weight PVDF-TrFE polymers. Moreover, a novel printable nanocomposite material, which allows reducing the cross-sensitivity between the pyro- and piezoelectric sensing modes, will be presented. This material is composed of inorganic ferroelectric nanoparticles blended in a ferroelectric polymer matrix. By exploiting the fact that the piezoelectric coefficient in inorganic ceramics has an opposite sign to that one of the ferroelectric polymer either the piezo- or the pyroelectric activity can be suppressed by independently defining the poling direction of particles and matrix in a clever poling procedure. Finally, applications such as flexible 3D user interfaces and large-area force, impact and proximity sensors will be presented.

OECTs in a lateral architecture are screen printed on A4 plastic substrates and investigated in view of a correlation between the electrical charge consumed during switching and the volume of PEDOT:PSS in the transistor channel. An understanding of the relation between charge consumption and the amount of electrochemically active PEDOT is essential for the design of high performance transistors and for providing a deeper insight into the fundamentals of the electrochemical switching process in OECTs. It turned out that a precise control of the width of the PEDOT:PSS source-drain line is imperative for maximizing both the on current and the on/off current ratio of lateral OECTs¹. In combination with screen-printed resistors, the printed transistors were also used as the building blocks for integrated logic circuits such as inverters, NAND gates, flip-flops, and a 2-bit shift register that operate at 1.5V. Only five different inks are needed to realize these circuits. Dynamic characterizations and comparison of 8 flip-flops (380 OECT and PEDOT:PSS resistors in total) reveal a remarkably high reproducibility of the measured devices' output signals, which is traced back to the high uniformity and stability of the basic building blocks. In this way, the suitability of PEDOT:PSS-based devices for integrated logic circuitry on flexible substrates by means of a low-cost printing technique is clearly shown².

In the last part first results in the context of active-matrix ferroelectric sensors combined with either an OTFT- or OECT-backplane will be presented.

¹ P.C. Hütter, A. Fian, K. Gatterer, B. Stadlober, Efficiency of the Switching Process in Organic Electrochemical Transistors, *ACS Appl. Mater. Interfaces* 2016, **8**, 14071–14076.

² P.C. Hütter, T. Rothländer, G. Scheipl, B. Stadlober, All Screen-Printed Logic Gates Based on Organic Electrochemical Transistors, *IEEE Trans. Electron. Dev.* 2016 **62**, 4231.

Charge transfer states for organic opto-electronics

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Intermolecular charge transfer (CT) states at the interface between electron-donating and electron-accepting materials in organic thin films are characterized by absorption and emission bands within the optical gap of the interfacing materials. 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 organic light emitting diodes, via thermally activated delayed fluorescence, while the latter property is exploited in organic photovoltaic devices and photodetectors. In this contribution, we will discuss the fundamental properties of CT states and link them to organic opto-electronic device performance. Furthermore, a new device concept will be introduced, using an optical cavity resonance effect to boost CT absorption at photon energies below the optical gap of both donor and acceptor, enabling narrow-band, near infrared (NIR) photo-detection. This new type of photodetector can compete with standard organic photodetectors but extends their detection range to longer wavelengths.

Novel Perovskite and Perovskite-inspired Materials for Solar Cells

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Hybrid lead iodide based perovskites (e.g. $\text{CH}_3\text{NH}_3\text{PbI}_3$) have recently demonstrated outstanding electronic properties and delivered impressive power conversion efficiencies in solar cells (>22%). However, practical implementation of this technology is hampered by several issues associated with such intrinsic properties of the complex lead halides as low photostability and high acute toxicity. Therefore, there is a constantly increasing interest to the development of principally new metal halides with non-perovskite crystal structure. Unfortunately, the best efficiencies reached for perovskite-like complexes based on Bi and Sb compounds stay below 1.5%.

In the present report, we will highlight the most recent results of our systematic study, which allowed us to demonstrate fairly stable all-inorganic perovskite materials and design the first perovskite-like complex metal halides delivering competitive performances in solar cells. In particular, external quantum (incident photon to collected electron) efficiencies of the best systems approached 50-80%, which is comparable to the reference perovskite solar cells. Discovering a new family of the lead-free metal halides with the perovskite-like structure enabling efficient operation of solar cells paves a route towards design of a new generation of light absorbers for emerging “perovskite-inspired” solar cells.

This work was performed in the frame of the Skoltech-MIT NGP program.

Oral talks

Polymer blends for precise control of electron and hole transport

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Ambipolar transistors are field-effect transistor (FET) devices in which the charge carriers can be both electrons and holes^{1,2}. In order to obtain ambipolar performances, the go-to approach usually is the use of two separate layers of the *p*- and *n*-type semiconductor, leading to ambipolar films. Regrettably, this approach requires complex processing methods (such as vacuum evaporation of the separate films) since the choice of solvent would be tricky if one was to process the films from the solution. Another approach is the use of ambipolar molecules. In most cases of ambipolar molecules, the $I_{\text{on}}/I_{\text{off}}$ was found to be much lower than in the case of hole or electron conducting molecules, due to high off current. Furthermore, there is very little control over the ratio between *p*-type and *n*-type mobilities, leading to often very unbalanced ambipolarity³. Here we report perfectly ambipolar transistors that could be fabricated using blends of *n*-type and *p*-type polymers. P(NDI2OD-T2) was blended with 4 different *p*-type polymers (P3HT, PCD-TPT, IIDDT-C3 and PDVT-8), and each time it was possible to fabricate devices with balanced *p*- and *n*-type mobilities. In particular, devices with mobilities over 10^{-2} cm²/Vs and linear regime $I_{\text{on}}/I_{\text{off}}$ over 10^5 were produced with a blend of P(NDI2OD-T2) and PCD-TPT. Impressive electrical performances obtained with PCD-TPT (a completely unbalanced ambipolar semiconductor) demonstrate that our approach can be used to adjust the electrical performances of ambipolar polymers featuring unbalanced mobilities (Fig. 1a). Furthermore, devices produced from P(NDI2OD-T2) blended with IIDDT-C3 featured mobilities up to 10^{-2} cm²/Vs and $I_{\text{on}}/I_{\text{off}}$ of 10^7 , unprecedented values for ambipolar organic transistors (Fig. 1b). In order to demonstrate this potential for applications, high performance inverters were fabricated for each material combination (Gain exceeding 100).

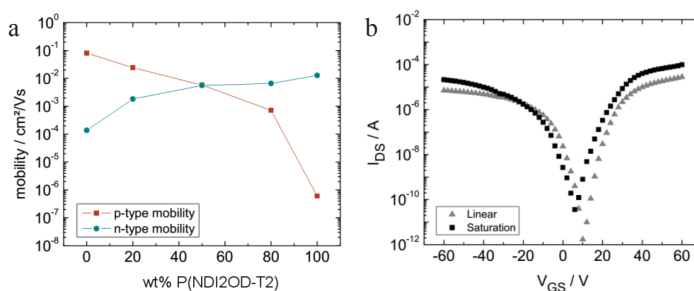


Fig. 1. Electrical characterization of films produced from P(NDI2OD-T2) blended with IIDDT-C3. (a) *p*- and *n*-type mobilities as a function of the percentage of the wt% of P(NDI2OD-T2) in the blend; (b) transfer curves of the 50:50 transistor.

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Graphene ferroelectric field-effect transistors: up-scaling and practicality

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Graphene is a two-dimensional material with many foreseen promises for opto-electronic applications. Chemical vapor deposition (CVD) of graphene on top of metallic foils is a technologically viable method of graphene production. Conventional photolithography and deposition of metal contacts on top of the transferred graphene layer to fabricate microelectronic devices is potentially invasive for graphene, and yields large spread in device parameters, and can inhibit up-scaling.

In this contribution, we demonstrate an alternative process technology in which both lithography and contact deposition on top of graphene are prevented. First a pre-patterned substrate is fabricated that contains all the device layouts, electrodes and interconnects. Then CVD graphene is transferred on top. Processing parameters are adjusted to yield a graphene layer that adopts the topography of the pre-patterned substrate. The metal-graphene contact shows low contact resistances below $1 \text{ k}\Omega \mu\text{m}$ for CVD graphene devices. The conformal transfer technique is scaled-up to 6" wafers with statistically similar devices and with a device yield close to unity. Conformal transfer is a generic process and can be applied for the transfer of any two-dimensional material.

Next, we demonstrated functional graphene devices, namely graphene ferroelectric field-effect transistors (GraFeFET) using the conformal transfer technique. As ferroelectric gate we used ferroelectric polymer, poly(vinylidenefluoride-trifluoroethylene) (P(VDF-TrFE)). Device processing was optimized to obtain robust, highly reproducible GraFeFETs that operates at both electron and hole accumulation regimes. We present further dual-gated GraFeFETs wherein the on/off ratio can be controlled by a second non-ferroelectric gate.

Finally, we present a model that captures the device physics of (dual-gate) GraFeFETs by incorporating the polarization of the ferroelectric gate. We predict, based on the model practicality of the graphene ferroelectric field-effect transistors.

Asymmetric Injection in OTFTs via Direct SAMs Functionalization of Electrodes

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The fabrication of organic opto-electronic devices integrating asymmetric electrodes is key in order to optimize charge injection/extraction at each individual metal/semiconductor interface for application in solar cells, LETs, OLEDs, inverters, photo detectors and sensors.¹ An alternative strategy to employing to different metals is the functionalization of gold with different thiols. Such functionalization of the Au electrodes is of pivotal importance, for locally controlling the charge injection at the organic-semiconductor interfaces.² Furthermore, the possibility of grafting specific functional units on Au electrodes is key for applications in (bio)sensing and multifunctional devices.³ Here we propose a new method for the asymmetric functionalization of gold electrodes⁴ with different thiolated molecules that allows us to obtain two electrodes with drastically different work function values. The procedure involves precise and ad-hoc micro-fabrications techniques, starting from the design of electrodes geometry. By constructing a specific (micro)-polymeric mask using a Laser Marker, we demonstrated that is possible to protect one electrode during the first functionalization step. PhotoElectron Yield-Counter Ambient Spectroscopy (PEYA) has been used to characterize the energetic properties of the asymmetrically modified electrodes, whereas X-Ray Photoelectron Spectrometry (XPS) provided a compositional confirmation of the successful asymmetric functionalization. Finally, we used poly(3-hexylthiophene) (P3HT) based organic thin-film transistors (OTFTs) to show for the first time, that the asymmetric electronic response stems from the different energetic alignment (stepwise and anti-stepwise) at the electrode's interface.

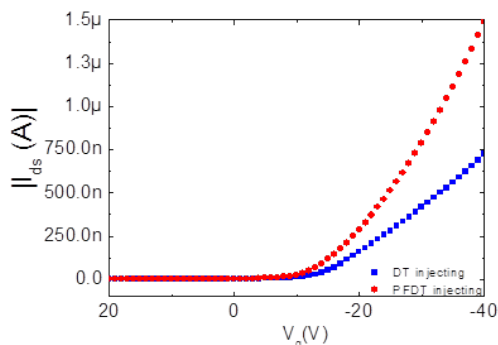


Fig. 1. Transfer Characteristics of the asymmetric OTFTs. In red is reported when injecting in an energetic stepwise configuration, in blue when injecting in an anti-stepwise configuration

This work was supported by the EC through the Marie Curie ETN project iSwitch (GA No. 642196).

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On the role of metal/semiconductor interfaces and of the density of states in the modeling of organic thin film transistors

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It is widely acknowledged that if injection/extraction phenomena are not accounted for, then the analysis of transfer characteristic curves of thin film transistors yields an apparent carrier mobility which is smaller than the intrinsic one. Recently, it has been reported that an improper treatment of experimental data may also lead to overestimating the mobility¹. In this contribution, we suggest that the situation is even more subtle and delicate. In fact, for a given experimental transfer characteristic curve in the linear regime, we find that the numerical fitting, and therefore the set of fitting parameters, are not unique. We model the mobility according to the Enhanced Gaussian Disorder Model and assume that source/drain contacts work in the current crowding regime. As a case study we consider a staggered transistor with gold contacts based on the prototypical n-type polymer P(NDI2OD-T2). Due to the uncertainty on the metal/semiconductor energy barrier Φ_B , this latter is a fitting parameter, which affects the magnitude of contact resistances. For each value of Φ_B , we determine the width of the Gaussian Density of States σ (and hence of the mobility) which yields the best fitting of transistor curves². We find that experimental curves can be equally well fitted by $\Phi_B = 0.7$ eV and $\sigma = 3.3$ kT, and by $\Phi_B = 0.54$ eV and $\sigma = 2.7$ kT, both set of values being, unfortunately, physically sound and plausible. To solve the degeneracy, the experimental framework has to be expanded so to include AC characterization in addition to DC characterization. Doing so, we find that only one set of parameters is acceptable, viz. $\Phi_B = 0.54$ eV and $\sigma = 2.7$ kT, whereas the one with the larger energy barrier results in a simulated frequency behavior showing a cut-off due to contact limitation occurring at too low frequency, at variance with experimental measurements. The value of 0.54 eV for Φ_B , smaller than the nominal one of about 1 eV (considering a LUMO of 4 eV and a gold work function of 5.0 eV) is in agreement with recent studies demonstrating that solvent-cleaned, contaminated gold surfaces (which is our case) show an effective work function of about 0.45 eV³.

Our work shows that the interplay between metal/semiconductor Schottky contacts at source and drain and the density dependent mobility, make transistor modeling a non-trivial task, and that DC measurement on a single device may be not enough to correctly identify fitting parameters.

This work was partially supported by ERC H2020, grant agreement 638059.

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Two-Step Nucleation in Solution-Printed Organic Semiconductors

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Two-step nucleation mediates the crystallization of a wide range of natural and synthetic products ranging from soft materials, such as proteins, bio minerals, colloids and pharmaceutical molecules, to inorganic compounds. Solidification in two-step nucleation proceeds via an intermediate amorphous state. In this contribution we show that two-step nucleation is operant during the solution processing of conjugated organic semiconductors (OSCs). This is demonstrated through *in situ* diagnostics of solution processing experiments, such as spin coating and blade coating. We go on to show that this nucleation mechanism can be controlled to achieve formation, in some instances, of high quality polycrystalline films by blade coating various OSCs in carefully designed processing conditions, resulting in highly textured and well-connected domains which exhibit reduced interfacial and bulk trap state densities, helping raise the carrier mobility by one to two orders of magnitude in organic field-effect transistors (OFETs). Solution printed OSCs such as 2,7-Dioctyl[1]benzothieno[3,2-b][1]benzothiophene (C8-BTBT) and 2,7-Di-tert-butyl-[1]benzothieno[3,2-b][1]benzothiophene (ditBu-BTBT) are thus produced at industrially compatible coating speeds i.e. 100 mm/s with carrier mobility $> 10 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ and minimal performance variability. The observation of two-step nucleation as a dominant phase transformation mechanism in OSCs and the ability to control its behavior during solution processing is expected to lead to important breakthroughs in organic electronics which often suffer from low performance and low reproducibility issues.

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Aligned and Region-Selective Deposition of Organic Nanowires for Thin Film Transistor Applications

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Organic semiconductors are promising candidates for solution-processed, large-area, low cost electronic devices. The patterning of organic semiconductors on the large scale is, however, challenging. Additionally, charge transport in organic semiconductors is typically strongly anisotropic, which leads to variations in the device performance if the semiconductor is not oriented¹. Therefore, the ability to control the alignment of the crystalline orientation of the semiconductors is highly desirable. Both, the patterning and the alignment of semiconductors can be achieved by a wetting/dewetting-based deposition on substrates with micropatterns of self-assembled monolayers (SAMs)^{2,3,4}.

Here we report on the aligned and region-selective deposition of organic semiconductor nanowires on SAM-patterned substrates, for thin film transistor applications. Organic semiconductor nanowires of dioctyl perylenebisimide (C₈-PDI) and hexathiapentacene (HTP) were grown by a solution-based method and dispersed into non-solvents. Substrates with micropatterns of SAMs with hydrophilic functional end group were prepared in a matrix of fluorinated SAMs to provide wettable areas in a non-wettable matrix. Upon doctor-blading of the nanowire dispersion, dewetting occurs in the fluorinated areas leading to a region-selective deposition of the nanowires in the hydrophilic areas. Beyond the mere patterning, an alignment of the nanowires was achieved by adjusting the dimensions of the wettable regions to be smaller than the length of the nanowires. This approach allows for the first time to efficiently pattern and align organic nanowires at the same time and thus incorporate them into transistor devices.

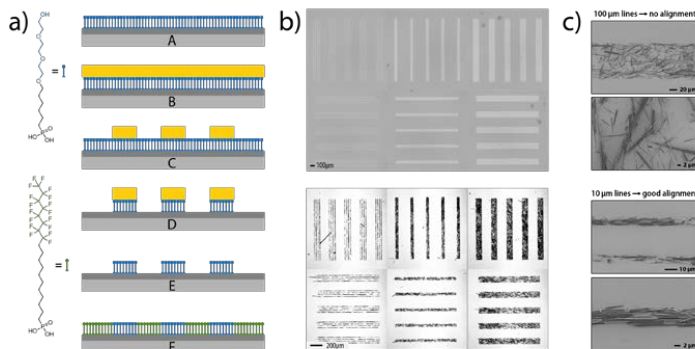


Fig. 1. a) Schematic process for the fabrication of SAM patterns; b) SEM images of SAM patterns before (top) and after (bottom) region-selective nanowire deposition. c) SEM images visualizing the effect of the width of the wetting pattern on the alignment of the nanowires.

This work was supported by the Alexander von Humboldt-Stiftung/Foundation.

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How many parameters actually affect the mobility of conjugated polymers?

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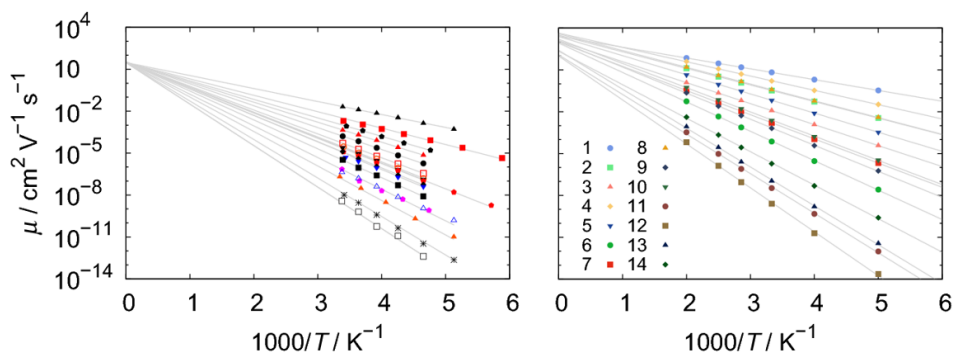


Fig. 1. Left: experimental charge mobility vs. $1/T$ for a range of organic semiconductors. Right: mobility vs. $1/T$ from our theoretical model with various amounts and types of disorder.

We describe charge transport along a polymer chain with a generic theoretical model depending in principle on tens of parameters, reflecting the chemistry of the material. The charge carrier states are obtained from a model Hamiltonian that incorporates different types of disorder and electronic structure¹ (e.g. the difference between homo- and co-polymer²). The hopping rate between these states is described with a general rate expression,³ which contains the rates most used in the literature as special cases. We demonstrate that the steady state charge mobility in the limit of low charge density and low field ultimately depends on only two parameters: an effective structural disorder and an effective electron-phonon coupling, weighted by the size of the monomer.⁴ The results support the experimental observation^{5,6} that the mobility in a broad range of (polymeric) semiconductors follows a universal behaviour, insensitive to the chemical detail.

This work was supported by EPSRC (EP/N021754/1) and ERC (Grant No. 615834).

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Fully Printed OTFTs: Fabrication and Large Signal Modeling

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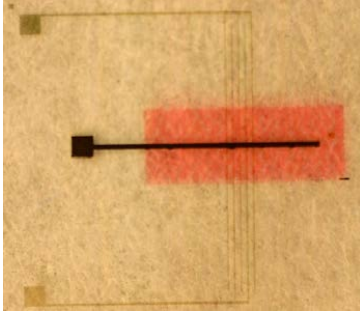


Fig. 1: Photograph of the fully printed OTFTs

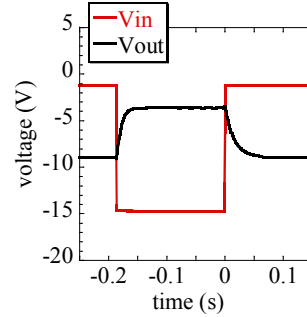


Fig. 2: measured output of a common source amplifier ($R_{load} = 100 \text{ M}\Omega$).

Organic electronics is rapidly evolving and considerable progress in organic thin film transistors (OTFTs) have been recently achieved. As one of the main expected advantages of organic electronics is the low cost, printing technologies are currently investigated as preferred processing techniques for the fabrication of OTFTs. In order to successfully design electrical circuits employing OTFTs, compact models that are able to precisely reproduce the DC as well as the AC behavior of these devices.

In this work, multi-fingered OTFTs, with staggered top-gate configuration (Fig. 1), were fabricated on PEN substrates by means of a fully printed process. Source (S) and drain (D) contacts were deposited by ink-jet printer and Ag nanoparticle ink. After SAM treatment of the contacts, semiconductor layer (30 nm thick Merck lisicon®SP400, formulated for gravure printing) and dielectric layer (Cytop CTL-809M, 400 nm thick). Finally, Ag gate electrodes were defined by ink-jet printer. Simple circuits (amplifier, inverters) have been realized by the above fully printed process.

OTFTs operating in AC regime (Fig. 2) have cut off frequencies of the order of few kilohertz and it is very likely that organic circuits used in practical applications are found to operate in a non quasi static (NQS) regime. Due to the large tolerance associated to printing processes, the layout of printed OTFTs includes large parasitic regions and their presence, that is negligible in DC operation, must be accounted in order to reproduce the AC behavior. In order to reproduce the AC behavior, a large signal non quasi static (LS-NQS) compact model, based on the variable range hopping (VRH) theory and on the current continuity equation, has been developed. In order to solve the resulting PDE, a discretization scheme based on a spline collocation approach is used, thus transforming in a set of ordinary differential equations (ODE) that has a straightforward circuitual analogous: it is very easy to solve the ODE system within a circuit simulation software environment such as a SPICE-like program or using the Verilog-A language. The model has been implemented in the Verilog-A language and has been validated by comparing the simulated dynamic characteristics with the experimental measurements performed on fully printed OTFT circuits

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X-Ray Imaging with Flexible Direct Organic Detectors

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Recently, the attention on the application of organic electronic materials for the detection of ionizing radiations is rapidly growing among the international scientific community. This is due to the great potential of the organic technology to envisage the need of large-area conformable sensor flat panels for applications that span from cultural heritage preservation to the security of public buildings. Indeed, organic materials are flexible and they can be easily deposited over large and bendable substrates by means of low-cost wet-technologies as printing techniques, overcoming thus the constraint of traditional inorganic materials, i. e. expensive or complex growth techniques and stiff mechanical properties.

In last years, our group reported about the employment of solution-grown organic materials as reliable direct X-ray detectors, operating at room temperature^{1,2,3,4}. These studies open the way to the development of a new class of fully flexible organic-based direct detectors with higher performances. Here we will report about our recent results on organic thin-films based, fully bendable, devices as direct X-ray detectors, with sensitivity values up to several hundreds of nC/Gy at ultra-low bias of 0.2 V⁵. An analytical model accounting for the signal amplitude and sensitivity values achieved has been developed. This allowed the realization and the demonstration of operability of a 2×2 pixelated matrix organic detector, providing the first full-organic X-ray imaging for real application.

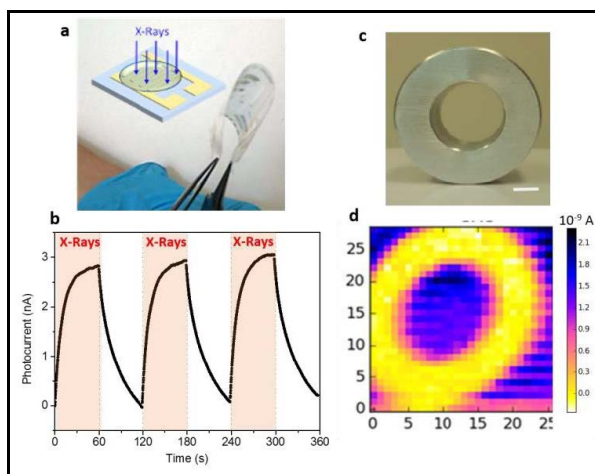


Fig. 1. (a) Image showing the flexibility of the structure and in the inset the schematic of the schematic of the device structure. (b) X-ray-induced photocurrent signal recorded at a bias voltage of 0.2V, upon three on/off switching cycles. (c) Photograph and corresponding X-ray image (d) of an aluminum annular ring; the scale bar is 5 mm.

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Efficient Triplet Exciton Fusion in Molecularly Doped Polymer Light-Emitting Diodes

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A strategy for raising the efficiency of a solar cell beyond the Shockley-Queisser limit is to harvest sub-bandgap photons via up-conversion. Such process is possible through the use of molecular upconverters based on triplet-triplet annihilation (TTA). On the other hand, formation of emissive singlet excitons via TTA (triplet fusion) is a route to increase the internal quantum efficiency (IQE) of fluorescent OLEDs beyond the 25% spin-statistical limit (up to a theoretical 62.5% threshold). Here, we report this process in solution-processed polymer OLEDs doped with commercially-available molecular emitters and/or singlet fission sensitizers, some of which are used as OLED emitters for the first time. From transient measurements we determine the ratio of delayed (triplet-fusion-generated) to prompt (directly-generated) electroluminescence to be as high as 60:40. We find peak external quantum efficiencies of ~6%, which we model to give IQEs of ~30%, representing the most efficient solution-processed OLEDs from these emitters. For rubrene, we report exceptionally high solid-state TTA-upconversion quantum yields of up to 23% (TTA-upconversion reaction efficiency of ~70%) at excitation power intensities well below 100 mW cm⁻² (1-sun equivalent).¹ We anticipate that current solid-state photon upconverters which use the same set of molecular semiconductors may reach similarly high efficiencies in the future.

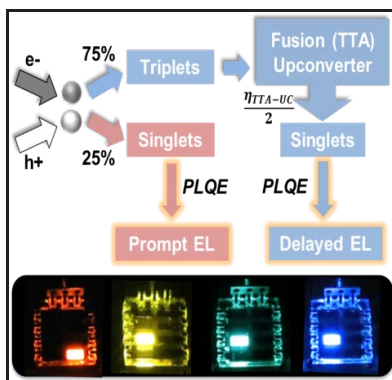


Fig. 1. Process illustrating triplet fusion in OLEDs and photographs of working multicolour OLEDs.

*This work was supported by studentship provided by A*STAR Singapore.*

¹ D. Di, L. Yang, J. Richter, L. Meraldi, R.M. Altamimi, A.Y. Alyamani, D. Credgington, K. Musselman, J.L. MacManus-Driscoll, R.H. Friend, *Advanced Materials*. 2016, in press.

Unravelling the Effect of Side Chain Environment in Conjugated Polymers Blends

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There is increasing awareness of the importance of side chains and their arrangement on the optoelectronic properties of conjugated polymers, due to their effect on backbone aggregation and particularly torsional disorder¹. Indeed, tailoring backbone functionality has become an established strategy to tune energy levels and device properties². By blending conjugated with insulating polymers, an approach that can enhance flexibility, reduce the amount of active material and tailor optoelectronic characteristics³, we control the interactions between side chains and their environment. Employing a range of structural and spectroscopic analytical methods, we explore the effect on microstructural and hence optoelectronic properties of matching the chemical functionality of the non-conjugated side chain to that of the insulator. Figure 1 shows initial evidence of increased aggregation and a temperature dependent return of vibronic structure in the blend, attributed to reduced steric hindrance from side chains. In summary, we demonstrate a new aspect of all-important structure-property relations in conjugated polymer blends, developing understanding of the factors affecting backbone conformation and hence excitonic coupling, with clear potential for tuning optoelectronic properties in a variety of devices.

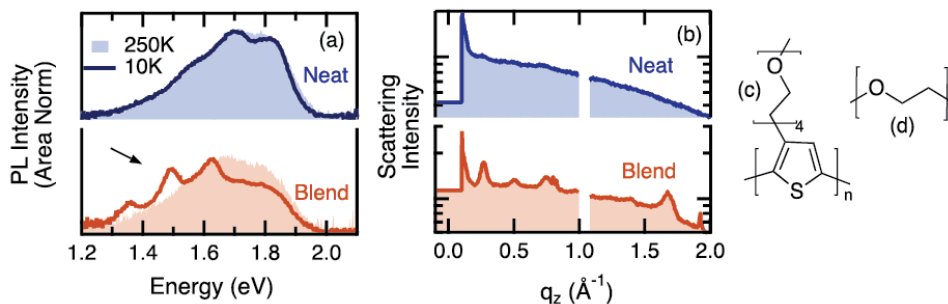


Fig. 1. Effect on photoluminescence (a) and grazing incidence X-ray diffraction (b) caused by blending poly(3-but(ethylene glycol-thiophene)) (c) with poly(ethylene oxide) (d), an insulating polymer with similar functionality to the side chains. Note the return of a vibronic progression in emission at low temperature in the blend, along with more pronounced scattering peaks indicating greater aggregation.

This work was supported by EPSRC, UK and ITN INFORM, EU.

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Boosting OLED efficiency by blending: spectroscopic identification of reduced charge trapping

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Many polymeric semiconductors of use in organic light-emitting diodes (OLEDs) are known to suffer from a strongly suppressed electron current due to the presence of trap states within the bandgap¹. As a consequence, the electron current density may well be several orders of magnitude lower than that of the positive charge carriers (holes). This unbalance in charge transport severely limits the operational efficiency of the device. An important loss process is so-called trap-assisted recombination, where holes non-emissively recombine with trapped electrons. Very recently², we have experimentally shown that if the traps are distributed in energy or sufficiently deep, their negative effect can be eliminated by spatially separating the charge accommodation sites via dilution of the semiconductor in an insulating host material, such as polyvinyl carbazole or polystyrene (PS)³. The observed increase in electron current and luminous efficiency validates long standing theoretical predictions.^{2,3} In this contribution, we present an analogous study based on the blue emitter poly(9,9-dioctylfluorene) (PFO), as it provides for the possibility of directly visualizing the reduction of charge trapping upon blending. This feature is obtained when the PFO contains a small fraction of fluorenone monomers, which represent emissive trap states whilst integrated in the polymer backbone⁴. Indeed, as observed in the electroluminescence spectra (Figure 1a) of corresponding devices, the broad green contribution associated with fluorenone emission can be fully eliminated upon blending the semiconductor with low molecular weight (~1 kDa) PS. Besides, current-voltage analysis of single carrier devices (Figure 1b) reveals that the electron current concomitantly rises due to reduction in both emissive and non-emissive charge trapping. For the blend containing only 10% active material the electron current approaches the hole current within two orders of magnitude. Our results show that by blending disordered emitters with affordable insulating materials, electron and hole transport become balanced, leading to increased OLED efficiency by reducing both the radiative and non-radiative trap assisted recombination. Hence, our method may pave the way to cost-effective large scale production of highly efficient OLEDs.

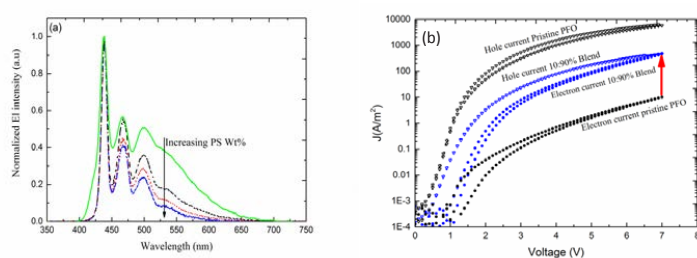


Figure 1. (a) Electroluminescence spectra of pristine PFO and PFO:PS blends in different weight ratios (b) Hole- and electron current density versus voltage for pristine PFO and PFO:PS blend with a 1:9 weight ratio.

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Charge separation and recombination in intermixed and “semi-planar” interfaces: PBTT-T/fullerene blends and solar devices

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The optimization of physical processes in organic solar cells is an established research area of utmost importance in the generation of sustainable and renewable energy. However, despite more than fifteen years of studies, a few issues are still not entirely understood in the field. One of them is the mechanism of charge separation and the factors that influence its efficiency.¹

In this work, we study the influence of the donor/acceptor interface nanostructure upon charge separation and recombination in organic photovoltaic devices and active blends composed of mixtures of PBTT-T and three fullerene derivatives with different blend ratios (PC₇₀BM, bis-PC₆₀BM and ICTA) as models for intermixed and semi-planar interfaces.^{2,3} Calculations of the free energy of interaction between a hole and an electron in the two interfacial scenarios result in important differences.⁴ While the completely intermixed system presents a monotonically increasing barrier for charge separation, in the planar interface this barrier disappears when energetic disorder is included in the model. We prove, with a combination of experimental studies including steady-state photoluminescence quenching (PLQ), fs-resolved transient absorption spectroscopy (TAS), and time-delayed collection field (TDCF) that systems with completely intermixed (1:1 PBTT-T/PC₇₀BM) or completely phase separated interfaces (1:1 PBTT-T/bis-PC₆₀BM and 1:1 PBTT-T/ICTA) result not only in low charge generation efficiency but also in extensive intensity-independent first order losses attributed to geminate recombination of bound charges. In contrast, the system that contains a combination of fully intermixed polymer/fullerene areas and fullerene phase-separated areas (1:4 PBTT-T/PC₇₀BM) results in slower, light intensity-dependent second-order recombination of free charges. We propose that small fullerene domains with low mobilities in the bis-PC₆₀BM and ICTA systems explain the kinetic-driven regime in which geminate charge recombination is dominant and translates in a low device performance.

This work was supported by the BMBF (13N1379), EPSRC (EP/IO1927B/1, EP/M023532/1, and EP/K011987/1), CONACyT (scholarship 309929) and the Kernahan Fund.

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Beyond the Shockley Equation: Reliable Parameter Extraction from Low-Mobility Organic Solar Cells

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The Shockley diode equation has been widely used to extract device parameters by modelling the current-voltage (J - V) characteristics of solar cells. Whereas this approach works well for silicon solar cells, it provides dubious parameters for devices based on low-mobility semiconductors. The diode ideality factor, n_{id} , and the dark saturation current, J_0 , are both intensity dependent and n_{id} increases with increasing intensity to physically inexplicable values $\gg 2$. For organic solar cells recently analytical diode models have been proposed which use $n_{id}=1$ and assume a reduced internal electric field due to the lower charge carrier mobility in these systems.^{1, 2} We have extended these diode models to incorporate additional series and shunt resistances and applied them for the first time to fit experimental J - V data of an organic solar cell (PTB7:PC₇₁BM) at various illumination intensities and temperatures. We took into account the temperature dependent charge carrier mobility³, obtaining directly from the new diode models J_0 and the intrinsic charge carrier density, n_i , which become intensity-independent and follow an Arrhenius function, with an activation energy of approximately the effective energy gap. Furthermore from these two parameters we could directly obtain the temperature-dependent bimolecular recombination rate constant and the Langevin reduction factor, k_L/k , a key quality parameter, with $k_L/k=30$ at 295 K. We demonstrate that this approach is very suitable to reliably extract device parameters from low-mobility solar cells and we will present a conclusive overview of the device physics of this prototypal low-mobility solar cell system.

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New Conjugated Connections and Substituents for Enabling Efficient Organic Materials for Photovoltaic and Transistor Applications

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Organic semiconducting materials are of the great importance for the development of modern high performing optoelectronic materials featuring low cost, compatibility with flexible plastic substrates, and simple roll-to-roll processing technologies. π -Conjugated Donor-Acceptor (D-A) polymers represents one of the most important class of organic semiconductors^{1,2}. Conjugation of donor and acceptor units in a polymer backbone renders a number of unique properties of D-A polymers: 1. Ability to fine tune HOMO and LUMO energy levels as well as energy gap between frontier orbitals of materials; 2. Stabilization of exciton formation; 3. Enhanced interplanar (interchain) interaction leading to better packing of the material. The choice of appropriate donor and acceptor is critically important for the construction of D-A polymer³. A large variety of electron rich thiophene based molecules used as donor units. On the other hand electron poor heterocyclic systems can be efficiently employed as acceptor units for D-A polymers.

Investigations centered on ethylene/acetylene moieties for creating new optoelectronic materials have been carried out for more than two decades⁴. When installed in a semiconductor core, the compact, electron-withdrawing, and rigid carbon – carbon triple bond can impart a number of desired properties including stabilization of the frontier molecular orbitals (HOMO and LUMO) and planarization of the conjugated backbone, reducing unfavorable steric interactions between in-chain π -blocks⁵. In contrast to ethynylene (alkyne) containing moieties, the 1,3-butadiynyl (acetylene) group has been barely studied. Here we report the synthesis of several alkyl-substituted 1,4-di(thiophen-2-yl)buta-1,3-diyne (R-DTB) electron-rich building blocks, functionalized with diverse solubilizing alkyl chains at the thiophene 4-position, and their incorporation into new copolymers with the electron-deficient thienyl- diketopyrrolopyrrole (TDPP) unit (Figure 1).

In the second part of the talk the effect of structural modification of the widely known and broadly used for high performing organic semiconductors thienyl- diketopyrrolopyrrole (TDPP) and naphthalenedicarboximide (NDI) building blocks via addition or/and removal of key substituents on the molecular structure, packing, and the charge transport will be discussed.

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Deigning Novel Heteroarene Molecules for Organic Electronics: Indolo[3,2-b]indole (IDID) and 1,5-Naphthyridine-2,6-dione (NTD) Derivatives

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Heteroarenes serve as a structurally and an electronically fascinating molecular platform for applications in organic electronics such as organic field-effect transistors (OFETs), organic light emitting diodes (OLEDs), and organic solar cells (OSCs). As one of the most promising heteroarenes backbone structure, fused pyrrole-containing ones have been investigated based on their strong electron donating nature and controllable π -conjugated system with high flexibility which are of great importance in view of electronic properties engineering. In this respect, among others, we have focused our interest on indolo[3,2-b]indole (IDID) backbone, which comprises two inner pyrrole rings and two outer benzene rings fused all together. We have synthesized structurally elaborated IDID derivatives for high-performance OFET with hole mobility of $0.98 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and versatile processability¹. Utilizing strong electron donating nature of IDID, intramolecular charge transfer (ICT)-type low bandgap small molecules for single-component ambipolar OFET and bulk heterojunction (BHJ) small molecular OSCs (SMOSCs) have also been developed². Halogenated IDID derivatives were newly synthesized and employed as the hole transporting layer of perovskite solar cell to give remarkable power conversion efficiency of $> 19 \%$ with long term stability³.

Planar bis-lactam-based materials, such as diketopyrrolopyrrole (DPP) and isoindigo (II) have attracted significant attention due to their high electron affinity driven by electron withdrawing nature of the lactam units, quasi-planar backbone structures, and the facile control over the molecular orbitals, which cooperatively yield outstanding charge carrier transport efficiencies in organic photovoltaics (OPVs) and organic field-effect transistors (OFETs). We have synthesized a novel electron-accepting bis-lactam building block, 3,7-dithiophen-2-yl-1,5-dialkyl-1,5-naphthyridine-2,6-dione (NTDT) and its derivatives. Compared to thiophenyl substituted DPP (DPPT), which has extensively been used as the most efficient bis-lactam unit, NTDT unit exhibits higher co-planarity of the conjugated backbone owing to the intramolecular S \cdots O interactions, deeper highest occupied molecular orbital energy level, and remarkably higher molar extinction coefficient. All these factors ensure that the NTDT unit is a promising electron-accepting building block for use in organic optoelectronic devices. We demonstrate that NTDT-based conjugated polymer exhibits outstanding power conversion efficiency of $> 9\%$ in the bulk heterojunction solar cells⁴.

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Conductive polyelectrolytes as a basis for a new generation of electronic devices

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It is now time of rethinking the whole set of experimental data on the behavior of various conducting polymers, which initially were considered promising for applications in organic electronics. Optimistic forecasts of the use of conductive polymers in real devices in the early 2000's gave way to a much more cautious statements about the possibility of niche applications. The main reason for the shift to cautious pessimism - low long-term stability of conductive polymers and their relatively high cost, due to the need for a multi-step synthesis. These disadvantages are not overbalanced by the advantages, such as the ease of manufacture using wet chemistry, tolerance to the atmosphere ambiente during application, variation of the properties of conducting polymers, the possibility of a predetermined change of their morphology.

However, against the general pessimism, there exist a number of areas in which the polymers do not duplicate inorganic electronics, but go own way, resulting in devices with no analogues on inorganic side.

The absolute leaders are polymer materials, having both high electron (hole) and high ion conductivity. The most promising classes of such systems are those, based on PEDOT and PANi, having high ion mobility as hybrid organic-inorganic interpolyelectrolyte complexes with inorganic dopants such as heteropolyacids, providing high proton conductivity and high electron or hole conductivity in the same material. These can also be in the form of interpenetrating networks and interpolyelectrolyte complexes of conductive polymers with polymers, containing ionogenic groups or nanoheterogeneous mixtures of PEDOT and PANi with polymers, providing high ionic conductivity by protons or Li⁺.

A separate series of anomalous properties appear, if one can create both polymers of p-type and n-type conductivity of this type and allow p-n homojunction, with the possibility of ion transport, that changes redox state of the polymer both at one and the other side of such homojunction. The ions movement along with electrons in such materials lead to peculiar phenomena, such as ionic Zeebek and reciprocal effects, anomalous piezoelectric properties etc.

The possibility of creating a new class of electronic devices, based on such materials, including piezoelectric and thermoelectric generators, memristors and neural networks will be communicated.

Donor-acceptor molecules with electron-withdrawing phenyldicyanovinyl groups for organic solar cells

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Donor-acceptor molecules of linear¹⁻⁵ and star-shaped¹⁻¹² architecture having alkyldicyanovinyl units as electron-withdrawing groups have shown a number of benefits as compared to pristine dicyanovinyl (DCV) groups. In this work, we extend that concept and design the triphenylamine-based star-shaped and unsymmetrical molecules having phenyl substituent at DCV group (Fig.1). The modification of DCV unit brings many positive changes to the physical properties of the molecules as compared to the analogs. It leads to a significant increase of thermal stability and solubility in organic solvents as well as higher crystallinity, while photovoltaic properties stays on similar or even higher level. Thus, both solution-processed and vacuum-deposited organic solar cells prepared from these donor molecules showed a power conversion efficiency up to 5%.

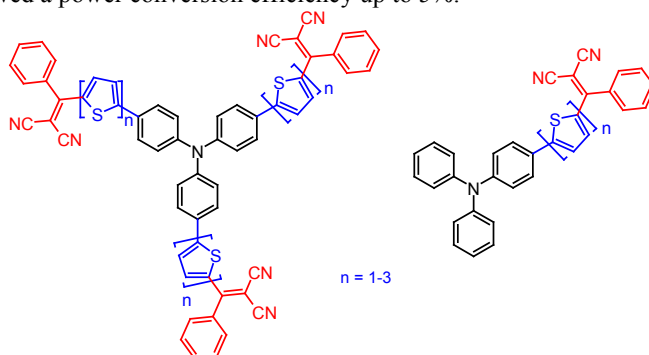


Fig. 1. Schematic representation of (a) star-shaped and (b) unsymmetrical TPA-based oligomers

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Highly-emissive 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 emission¹. One of the most useful routes for increasing luminescence is furan incorporation, which also yields an additional benefit of increased molecular rigidity and solubility highly favorable for industrial applications^{2,3}. In this work, we studied single crystals of furan/phenylene co-oligomer 1,4-bis(5-phenylfuran-2-yl)benzene (BPFB, Fig. 1a) combining high photoluminescence quantum yield (PL QY) with efficient charge transport.

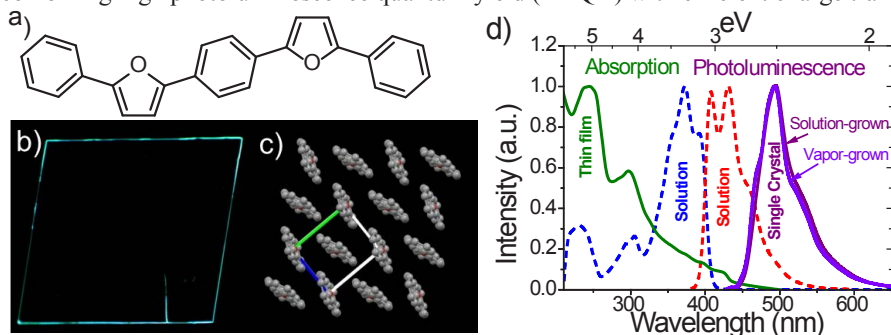


Fig. 1. a) Chemical formula of BPFB; b) Optical image of BPFB single crystal in UV light (405 nm); c) Herringbone packing of BPFB molecules in the plane of the main crystal face; d) Optical spectra of BPFB samples: absorption in solution (dashed blue) and thin film (olive); photoluminescence in solution (dashed red) and single crystals grown from solution (purple) and vapor (violet).

The crystals were grown by conventional physical vapor transport technique as well as by solvent-antisolvent crystallization to compare charge transport and luminescence properties. BPFB molecules have herringbone packing (Fig. 1c) with the long molecular axis being almost perpendicular to the main crystal facet which corresponds to H-aggregation. Whereas both types of crystals demonstrate the same charge mobility $0.1 \text{ cm}^2/\text{Vs}$ solution-grown crystals have PLQY as high as 60% nearly 1.5 times surpassing vapor-grown ones. Such a combination of high PL QY with good charge transport demonstrates that solution-processable furan/phenylene co-oligomers are promising materials for organic optoelectronics.

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Structure and complex formation properties of hemicyanine chromoionophore monolayers for sensor applications

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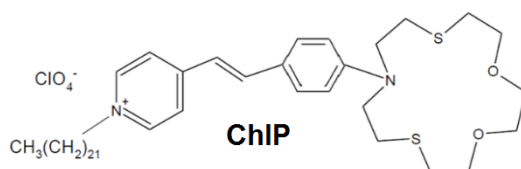
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Hemicyanine dyes attract special attention due to their spectral characteristics and possibility to easily impart required properties to these compounds via chemical modification of terminal groups. In the present work, a hemicyanine dye was functionalized by dithio-aza-crown-ether group, which can selectively bind mercury ions, and an alkyl “tail”, which provides amphiphility to the chromoionophore molecule (ChIP).



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 Hg^{2+} 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. Thus, presence of mercury ions in the subphase under the studied monolayer leads to formation of 1:1 type complexes (one analyte ion per one ChIP molecule) and 1:2 complexes, in which two ChIP molecules are coordinated by one mercury cation and which do not exist in solution. This cation binding leads to noticeable changes of dye monolayer absorbance and fluorescence spectra as well as X-ray reflection patterns. It was established that presence of barium cations in the subphase inhibits the head-to-tail aggregation of ChIP molecules in the compressed monolayer. 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. Changes of both structure and sensitivity of the ChIP monolayer to the analyte in the subphase were confirmed by fiber optic absorbance and fluorescence spectroscopy combined with X-ray reflectivity measurements performed simultaneously using synchrotron radiation. It was 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, 16-29-05272 and ESRF S4447.

Poly(3-hexylthiophene) nanoparticles containing thiophene-*S,S*-dioxide: tuning of dimensions, optical and redox properties and charge separation under illumination

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Recently, we have successfully demonstrated that through an opportune chemical strategy - based on the oxygenation of thiophene sulphur atom with Rozen's reagent - it is possible to prepare poly(3-hexylthiophene) nanoparticles containing thiophene-*S,S*-dioxide units (TDO) either randomly distributed in the NPs (PTDO-NPs) or located only in the outer layer forming all-organic *core-shell* nanoparticles (P3HT@PTDO-NPs) (Fig. 1)¹. We proved that through controlled insertion of TDO moieties it is possible to achieve an unprecedented tuning of NPs size, which can be scaled down to 5nm, and of NPs chemical-physical properties such as a markedly low-lying LUMO (in the range 0.5-0.9 eV), a very low energy gap (1.43eV) and a change from p- to n-type semiconducting behavior as inferred from Kelvin Probe measurements. Finally, we demonstrated that the coexistence of p- and n-type charge carriers in TDO containing nanoparticles allows for a marked charge separation under illumination, suggesting potential application in photovoltaic devices.

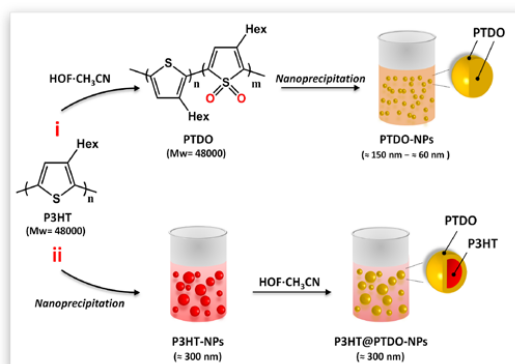


Fig. 1. Different strategies combining Rozen's reagent (HOF·CH₃CN) and nanoprecipitation techniques to get well-defined functionalized TDO-nanoparticles.

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Vacuum Deposition of Perovskite Layers – A New Tool Concept

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Perovskites are a special class of materials. The material properties of perovskites allow for a wide range of applications, their application in thin film photovoltaics (PV) is the reason for current interest in this field. Solar cell efficiencies of devices using these materials have increased from 3.8% in 2009¹ to 22.1%² in early 2016, making this the fastest-advancing solar technology to date. Recent publications demonstrate that perovskite PV could even reach a theoretical peak efficiency of 31%³. The deposition of the required thin film can be realized by a solution based processes, or via physical vapour deposition under vacuum conditions. As both processes have their own advantages, a clear favourite for the intended mass production is not yet evident.

Depositing these materials involves a co-evaporation of an organic precursor (organic halide, e.g. Methylammonium iodide) and an inorganic precursor (metal halide, e.g. Lead(II) iodide). While the Inorganic precursor can be simply evaporated in high vacuum, the organic precursor typically behaves “vapour-gas-like” due to its low molecular weight. Hence, heating the organic precursor source leads to a strong increase of the chamber partial pressure and to the deposition of the material on all chamber surfaces. Consequently, controlling the deposition rate of the organic precursor on the substrate is difficult.

To reclaim full process control, we designed a specific deposition system for perovskite layers based on a novel concept (patent pending). This system does include modifications to ensure long system lifetime. In addition, we developed a special deposition source for the organic halide compounds. Together with our novel system design, we are able to improve process control, resulting in a higher repeatability of subsequent depositions. Furthermore, we give the operator an additional lever to fine-tune the perovskite deposition using controlled multisource co-deposition, making our system the ideal tool for efficient R&D in this vivid field (e.g. band gap tuning).

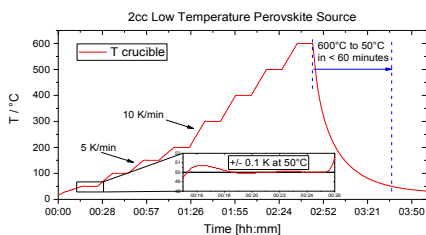


Figure 1: Defined source temperature control



Figure 2: CreaPhys application lab

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² Certified (KRIT and UNIST); NREL Efficiency Chart.

http://www.nrel.gov/ncpv/images/efficiency_chart.jpg

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The interface charge transfer and the energy level alignment upon vacuum deposition of the ultra-thin conjugated molecular layers onto solid surfaces

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The interface charge transfer and the energy level alignment in all-organic and in organic/inorganic interfacial structures is a subject of a great scientific interest due to the possible electronic device applications. The analysis of the phenomena related to the intermediate layer formation at the interface can be used to tune the electronic structure of the organic materials and for control of the charge carrier injection^{1,2}.

In the present work the electron spectroscopy techniques such as total current spectroscopy (TCS) and dissociative electron attachment spectroscopy (DEAS) were used to characterize the electronic properties of the conjugated molecular films on solid surfaces and electron attachment to vacant orbitals of the isolated molecules. The first-principle theoretical calculations were conducted to support the experimental findings. The atomic force microscopy (AFM) and the X-ray photoelectron spectroscopy were used to control the film structure and the atomic composition. The interfacial charge transfer and the density of the unoccupied electronic states (DOUS) were studied at the all-organic interfaces of the hexadecafluoro copper phthalocyanine and the unsubstituted copper phthalocyanine, the dinitro substituted and unsubstituted phenylene-vinylene oligomers, bisimide substituted perylene based molecules and at the interfaces of these films contacting the silicon oxide surface.

The substantial changes of the DOUS peak structure in the energy interval of the π^* and the low-lying σ^* orbitals were observed at the interface region between the ultrathin layers made from the substituted and the unsubstituted molecules under study³. 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 the electronic processes which occur at the interfaces the formation of the 1-2 nm thick intermediate layer of ionized molecules according to the integer charge transfer model⁴ and molecule fragmentation in the overlayer are considered.

The work was supported by RFBR grants 17-03-00196 and 15-29-05786. The XPS and the AFM measurements were performed at the Centre "Physical methods of surface investigation" and at the "Centre for Diagnostics of Functional Materials for Medicine, Pharmacology and Nanoelectronics" of the Research park of St. Petersburg State University.

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Flexible self-standing organic supercapacitors of carbon nanotubes/polypyrrole based on eggshell membranes

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The increasing use of portable devices and the upcoming internet of things represent a revolution in our life-style that relies on the continuous development of novel electronic gadgets. To enhance the autonomy of such devices, new types of energy efficient batteries and supercapacitors (SC) are necessary¹. In this work, we propose eggshell membranes (ESM) as a platform for the development of flexible SC based on the combination of carbon nanotubes (CNTs) and intrinsically conducting polymers. For that end, we exploited the three-dimensional porous structure of the ESM, whose proteins exhibit a large number of functional groups², to electrostatically assemble oxidized CNTs and polypyrrole (PPY) chains in such a manner as to create self-standing electrodes. Using a H₃PO₄-PVA separating layer, we have constructed and optimized a flexible SC, whose electrochemical properties were characterized. The optimized device presented a specific capacitance of 400 F.g⁻¹ [200 F.g⁻¹] when only the amount of active material [the whole SC] is considered. The typical capacitance of this novel type of SC displayed good retention properties (80% of the original value after 2000 operational cycles) and exhibit only a slight variation even after the whole device was bended more than 500 times. These results suggest that eggshell membranes, a usually discarded biomaterial, represent a promising platform for the development of electroactive nanostructures and the tailoring of a new family of sustainable SC.

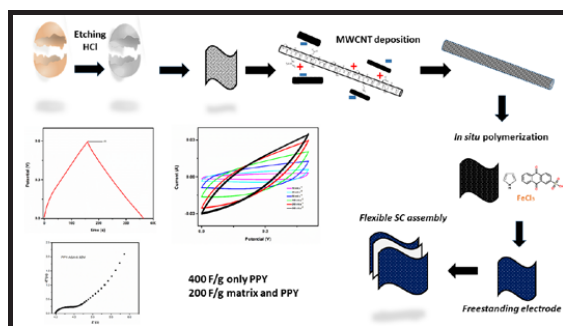


Fig. 1. Schematic representation of PPY-CNT ESM supercapacitor and its typical charge-discharge, cyclic voltammetry and electrochemical impedance characteristics.

This work was supported by the Brazilian agencies CAPES, FACEPE, INFO-MCTI, FAPESB, FINEP and CNPq.

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Nanopatterning conjugated polymers by laser: Influence on electrical properties

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Efficient polymer solar cells (PSCs) typically employ a bulk-heterojunction (BHJ) photoactive layer, where an electron-donating (p-type) phase and an electron-accepting (n-type) phase form a phase-separated interpenetrating network. This network can provide large enough heterointerface areas for efficient exciton dissociation and a continuous pathway for charge transport. Therefore, increasing the interfacial area between the e-donor and e-acceptor phases and limiting the morphology of the heterojunction to the nanoscale are critical for improving the device performance¹.

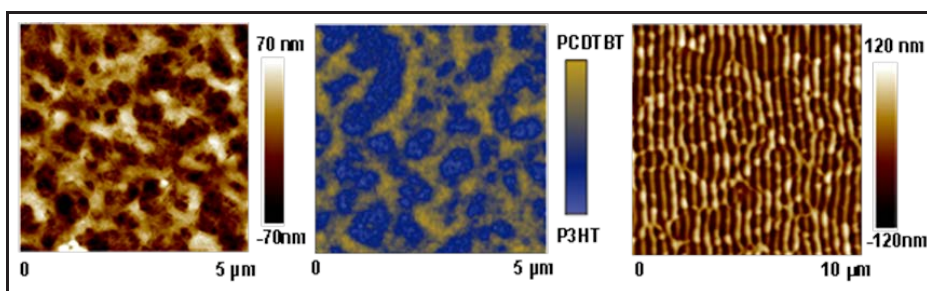


Fig.1. P3HT:PCDTBT (1:1) blend: AFM topography (left). Scanning transmission X-ray microscopy derived composition image (center). AFM topography of LIPSS (right).

In this contribution we will report on the structure-property or structure-performance relationships in all-polymer heterojunctions based on blends of poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3' benzothiadiazole)] (PCDTBT) and poly-3-hexylthiophene (P3HT)². In order to control the polymer structure at the nanoscale and to reduce the characteristic lengths of the OPV device toward the exciton diffusion length optimal limit, we have nanostructured the active layer by Laser Induced Periodic Surface Structures (LIPSS). In the case of polymers, several studies have shown that irradiation by a linearly polarized laser beam induces self-organized ripple structure formation within a narrow fluence range well below the ablation threshold³. We have proven the possibility of inducing LIPSS in conjugated homopolymers and blends as shown by atomic force microscopy (AFM) (figure 1, right). Near edge X-ray absorption fine structure (NEXAFS) and Raman spectroscopy measurements reveal good chemical stability of P3HT, PCDTBT and the blend thin films under the laser irradiation conditions used for LIPSS formation. Conductive atomic force microscopy (C-AFM) has been used in order to correlate structure and electrical properties for nanostructured systems³.

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Self-doping controls luminescence in thiophene-phenylene single crystals

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Emerging organic light-emitting electronic devices such as organic light-emitting transistors and lasers need materials combining high luminescence and efficient charge transport. The latter requires tight molecular packing, which commonly weakens the luminescence. Doping of the materials by highly luminescent molecules is an efficient approach to control and enhance the material luminescence. Here, we introduce the concept of self-doping according to which a higher luminescent dopant emerges as a byproduct in the course of the host material synthesis, and demonstrate how the dopant controls the luminescence of organic semiconducting crystals.

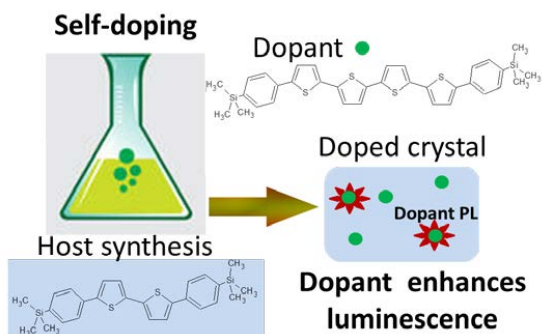


Fig. 1. Schematics of the self-doping concept.

As the host material, we synthesized thiophene-phenylene co-oligomers (TPCO) with the conjugated cores PTPP (P and T stand for phenylene and thiophene rings, respectively) with various end groups by using different synthetic routes. The TPCO crystals were grown from the vapor phase and solution. The dopant content was controlled by luminescent and photothermal deflection spectroscopy. Figure 1 exemplifies schematics of self-doping for the TMS-P2T-TMS/TMS-P4TP-TMS host-dopant system. We show that the photoluminescence (PL) in the doped single crystals is controlled by efficient Förster resonant energy transfer (FRET) from the host TPCO to the higher luminescent TPCO dopant. For TMS-P2T-TMS/TMS-P4TP-TMS host/dopant single crystals, the optimal doping level is about 1%, at which all PL comes from the dopant. Time-resolved PL data and Monte-Carlo simulations indicated that the Förster radius and the exciton diffusion length in the TMS-P2T-TMS/TMS-P4TP-TMS crystals are close and about 3 nm. We conclude that self-doping is a promising route to control and enhance luminescent properties of organic semiconducting materials.

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Thiophene-Based Single Crystal Monolayers for Organic Field-Effect Devices

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Single-crystal organic field effect transistors (OFETs) can provide electrical performance exceeding that of a-Si devices. Solution processing is one of advantages of organic electronics allowing low production costs. For industrial processing of organic single crystals, their high morphological homogeneity and thickness uniformity on large areas are needed. As charge transport in OFETs occurs within a few monolayers of organic semiconductor, ultrathin devices are beneficial from the viewpoint of low material consumption, mechanical flexibility and optical transparency. Herein, we report on solution-processed oligothiophene-based single crystal monolayers with sizes up to a few mm and study their performance as OFET active layers. As materials we used oligothiophenes and oligothiophene-phenylenes with five conjugated rings and different terminal alkyl substituents. Single crystal monolayers were grown on various substrates and studied by optical polarization microscopy, atomic-force microscopy, spectroscopic ellipsometry, and X-ray diffraction. Linear dimensions of thiophene-based single crystal monolayers reached 1-3 mm (Fig. 1a). Typical thickness of the crystals was (3.2 ± 0.3) nm, which was close to the lengths of oligomers (Fig. 1b). The OFET mobility of the best devices (Fig. 1c) exceeded by an order of magnitude the highest reported mobilities for oligothiophene-based monolayer OFETs¹. Thus, large-area solution-processed single crystal monolayers can be a promising platform for ultrathin organic electronic field-effect devices.

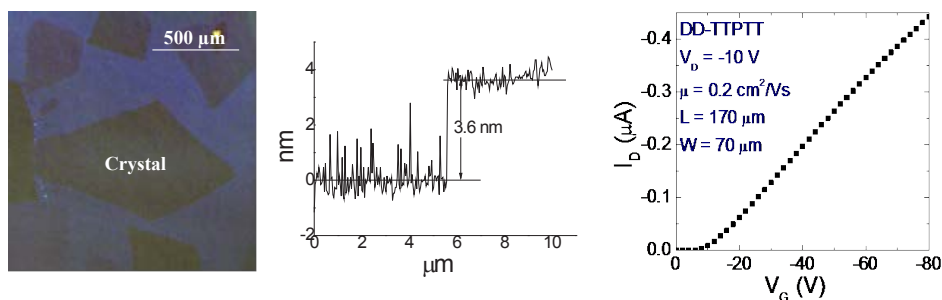


Fig. 1. Microscopy image of thiophene-based single crystal monolayers (a); AFM profile for thiophene-based single crystal monolayers (b); transfer characteristics in linear regime of OFETs based on thiophene-phenylene single crystal monolayers (c).

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

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Nanostructured organosilicon luminophores for 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 luminophores¹. 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 range⁸. 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 devices¹⁰.

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 364.2017.3).

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All PEDOT:PSS Organic Electrochemical Transistor for the selective detection of redox-active molecules in biological fluids

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Organic electrochemical transistors (OECTs) have been proposed as biosensors for redox-active biomolecules thanks to their remarkable features such as signal amplification, very low operating potentials and adsorbed power. Nevertheless, the lack of selectivity hinders their widespread use in real-life applications.

The selective detection of dopamine (DA), one of the most significant neurotransmitters in biological organisms, is currently a subject of significant interest. The rapid and accurate determination of DA is of great importance in the diagnosis of neurological disorders, such as Parkinson's disease, autism, schizophrenia. However, the main problem related to the electrochemical detection of dopamine is that its oxidation potential is close to that of other endogenous substances such as uric acid (UA) and ascorbic acid (AA), which leads to poor selectivity and sensitivity in DA detection.

We explored a new approach to selectively identify and determine the contributions of different analytes to the OECT electrical output signal through a potentiodynamic approach, by varying the operating gate voltage and the scan rate.

A selective all PEDOT:PSS OECT has been developed with sensitivities and limits of detection comparable or even better than those obtained by Differential pulse voltammetry, a technique that employs a sophisticated read-out system that can hardly be considered a viable method in practical applications.

The here reported OECTs exhibit very appealing features for wearable sensors: 1) the operating potentials are very low (< 1 V), a key point considering that the device must be placed in direct contact with skin; 2) since the current used as signal is quite high (~ 1 mA), it requires a simple readout electronics; 3) the absorbed power is very low ($\sim 10^{-4}$ W); 4) it can be deformed without observing a degradation of its electrical features.

Finally, we have fabricated all-PEDOT OECTs also by direct printing onto textile substrates, and we assessed the stability of the developed fully textile OECT under washing conditions

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Injectable, self-opening, and freestanding retinal prosthesis for fighting blindness

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Worldwide 190 million people are severely visually impaired, and about 32 million are blind¹. In Europe, macular degeneration and glaucoma are considered the leading causes of vision loss. Blindness is a widespread global public health issue, representing a significant personal and societal burden, limiting educational opportunities, affecting economic possibilities and reducing the quality of life^{2,3,4}. Although various approaches have been attempted so far, including drug treatment, gene therapy, stem-cells transplantation, optogenetics, and visual prostheses, with encouraging results in animal models and some also in patients⁵, there is still no established method to restore sight. Among those, retinal prostheses succeeded in restoring a primitive form of vision^{6,7}, such as locating and recognizing objects. However, fighting blindness with retinal prostheses requires challenges not yet achieved: implanting a prosthesis (i) large enough to cover the retinal surface and (ii) embedding a high number of highly dense stimulatory elements. We developed an injectable, self-opening, and freestanding prosthesis restoring at least 40° of visual field, therefore covering at least a retinal surface of 12 mm in diameter. Moreover, it has a hemispherical shape in order to minimize the distance from the targeted cells over its entire surface. It also operates according to a photovoltaic stimulation principle and it should be injected through a minimal scleral incision. Our implant is based on PDMS as shell material, embedding 2345 organic photovoltaic stimulating pixels made of conjugated polymers (100 µm and 150 µm in diameter, density 54 px/mm²), covering an active area of 13 mm (44° of visual field). Our results indicate that those pixels can deliver up to 54 mA/cm² and generate an electrode potential up to 200 mV when illuminated with a pulse light of 10 ms, 32 µW/mm², at 530 nm. Accelerated aging tests and experiments with explanted retinas are currently under evaluation. These preliminary results show the potential of organic photovoltaics in the fabrication of a retinal prosthesis with large area and high stimulation efficiency. The biocompatibility and mechanical compliance of the materials represent a step forward in building advanced photovoltaic retinal prostheses.

This work was supported by EPFL and European Commission (project № 701632).

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Characterization of organic semiconducting nanoparticles and their *in vitro* application

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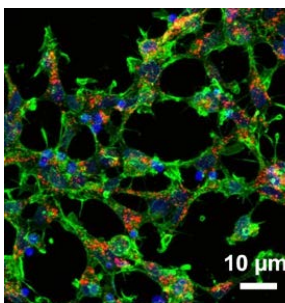


Fig. 1. Poly(3-hexylthiophene) nanoparticles interfacing with living cells: a new tool for biophotonics applications

In the last decades, searching for new multifunctional nanoscale materials with healthcare potential applications is remarkably impacting on biotechnological field. Among others, conjugated polymers gained attention for their applications in biosensing, bioimaging and drug delivery. Not only do they have intrinsic high biocompatibility, but they can also be exploited as light sensitive actuators by virtue of their photophysical properties.^{1,2}

In this work we investigate the possibility of taking advantage of poly(3-hexylthiophene) nanoparticles (P3HT-NPs) in biophotonics.³ We report on the synthesis of P3HT-NPs by reprecipitation method with excellent colloidal stability in aqueous solution under sterile conditions. We extensively characterize their photophysical properties in different media, including buffer and extracellular solutions, by time-resolved photoluminescence analysis. P3HT-NPs are then incubated with Human Embryonic Kidney (HEK) cells and their effective internalization is assessed by confocal imaging. Finally, we report a detailed study of the interaction between internalized nanoparticles and living cells, based on UV-VIS absorption, cytotoxicity experiments, immunofluorescence assays, calcium imaging and electrophysiology.

This work was supported by EU (project № FP7-PEOPLE-212-ITN316832-OLIMPIA), by grants Telethon – Italy (project № GGP12033 and GGP14022), and by National grant from Fondazione Cariplo (project ON-IRIS № 2013-0738).

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Single-substrate integrated active-matrix pyro-sensor

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We present the development, manufacture, and performance of a novel device consisting of a pyro-sensor based on our PyzoFlex[®] Sensor Technology integrated with active matrix electronics on a single flexible substrate. The technology is a step towards large area sensor devices, such as e.g. proximity-skin, merging flexible sensors and electronics exploiting the active matrix concept.

The ability of an organic transistor to switch a ferroelectric sensor is demonstrated, where the sensor detects an approaching human hand at distances up to at least 20 cm and the transistor is capable of switching frequencies in the range of several kHz. Consequently, the integration on a single large area flexible substrate is conceived and carried out applying only 4 shadow-mask and 2 screen-printing processes for patterning.

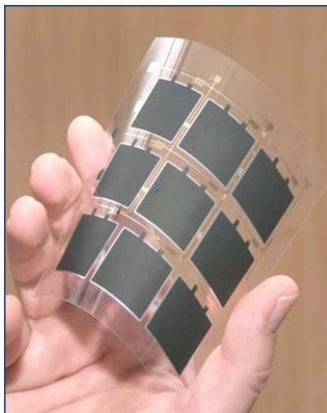


Fig. 1. A photograph of a 3x3 active-matrix pyro-sensor on a 12x12 cm² substrate

A 3x3 active-matrix on a 12x12 cm² substrate integrating transistor gate and bottom contact of the sensor as well as sensor-layer and a thick second dielectric for bus-line crossings is manufactured and electrically tested showing sensor action as in the single device test.

Financial support by the Austrian Bundesministerium für Verkehr, Innovation und Technologie (bmvit) is gratefully acknowledged.

Eumelanin-based electrodes for ITO-free devices in bioelectronics and nanomedicine.

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In the scenario of indium scarcity the blend of poly(3,4-ethylenedioxythiophene) with the poly(styrenesulfonate) (PEDOT:PSS) is a very promising candidate for the next generation of transparent electrodes materials. Nonetheless PEDOT:PSS does exhibit some limitations,¹ including the relatively low adhesion² particularly on inorganic substrates³ and low stability to water hampering full exploitation in bioelectronics eg. as material transducing signals across the biotic/abiotic interfaces⁴. Among bioinspired materials for functional biocompatible interfaces, the human pigment eumelanin is currently gaining increasing interest. This black insoluble pigment of human skin, hair, eyes and nigral neurons (neuromelanin),⁵ arises biogenetically from the aminoacid tyrosine via the oxidative polymerization of 5,6-dihydroxyindole (DHI) and/or 5,6-dihydroxyindole-2-carboxylic acid (DHICA)^{5,6}. Eumelanins feature unique assortment of chemical physical properties.⁶ Two main obstacles hampered a full exploitation of eumelanin based devices: (i) the actual eumelanin insolubility in any solvents, preventing easy processability of the pigment as well as the devices fabrication; (ii) its low conductivity, limiting both the range of possible working potential and functional applications. To improve the electrical performances of the eumelanin thin films, a clear-cut approach lies in the hybridization with a suitable conductive counterpart. In this view, π -conjugated molecules featuring conductive pathways appear a key choice in the production of new organic materials for electronic (nano)devices.

Here, we present the first preparation of an eumelanin-PEDOT blend (Eu-PH), featuring valuable functional and processing properties, like easy films preparation, high adhesion, good electrical conductivity and biocompatibility. The hybrid was characterized by chemical, physical, electrical and morphological analysis. The biocompatibility and toxicity was investigated in view of its potential exploitation as bio-interface material.

Finally, as a proof of concept, ITO-free organic light emitting devices, featuring Eu-PH as the anode and presenting performances comparable to reference ITO-free devices were fabricated and characterized.

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Bacterial cellulose modified with conducting and light-emitting polymers for organic biosensors applications

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Development of biocompatible nanochips on the basis of functional organic and polymeric materials and their composites is an important direction of current research in the field of medicine and organic electronics. Nanocellulose films as well as their composites with organic or inorganic components are widely used in modern medicine as nondrying membranes, artificial blood vessels, the material for tissue reconstruction, cartilage and bone tissue, and as bioelectronics devices - insulating substrates for organic light emitting diodes, field-effect transistors and biocompatible sensors. We have developed a new multifunctional composite materials based on films of bacterial cellulose (BC) modified with conductive polymer complex - PEDOT/PSS^{1,2}, as well as by semiconductor light-emitting polymer MEH-PPV³. The structural, electrical and optical properties of these hybrid materials have been investigated in the temperature range 310 - 77 K. It was shown that BC:PEDOT/PSS and BC:MEH-PPV films (thickness ~ 10 - 60 μm) have well pronounced fibrillar structure with a large number of pores, while the surface of BC fibrils is coated by conductive polymers PEDOT/PSS, MEH-PPV. The BC:PEDOT/PSS films characterized by strong absorption in the red and near-infrared spectral region while BC:MEH-PPV films demonstrate strong absorption in the ultraviolet region of the visible spectrum. BC:PEDOT/PSS films have a very low intensity of the photoluminescence (PL) at 300 K, while BC:MEH-PPV films characterized by a very strong PL and electroluminescence (EL) in the spectral range of 400 - 700 nm. It was found that the dependences of the EL intensity of BC:MEH-PPV films versus applied pulse bias and pulse frequency are rather strong and superlinear³. The temperature dependence of the resistivity of films BC:PEDOT/PSS follows a power law in the temperature range 310 - 77 K, while the resistivity of such composite films varies little over time¹. The dominant mechanism of charge carrier transport in BC:PEDOT/PSS and BC:MEH-PPV composite films is tunneling and charge transfer in the conducting polymer components: PEDOT/PSS and MEH-PPV respectively. Terahertz response of BC:PEDOT/PSS films has been studied by terahertz time domain spectroscopy². Spectra of refractive index, extinction coefficient and complex dielectric permittivity are obtained in spectral range of 0.3–2.8 THz for f BC:PEDOT/PSS films have been obtained. Considerable increase in the imaginary part of dielectric permittivity of BC:PEDOT/PSS films as compared to that of pristine BC film was found out. The results indicate the possibility of using BC:PEDOT/PSS composite films as a flexible biocompatible temperature and electrical sensors, while BC:MEH-PPV films can be used as transparent, flexible, biocompatible light-emitting paper (markers). The possibility of using BC:PEDOT/PSS and BC:MEH-PPV composites as materials for tissue engineering and 3D printing for bioelectronics is discussed.

This work was partially supported by RFBR (project № 15-02-01897) and PRAS No 1.8P.

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Highly sensitive gas sensors based on LS OFETs

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Nowadays development of portable, highly efficient, selective and low cost gas sensors working at ambient environment with fast response and long lifetime is one of the challenges for modern electronic industry. The range of potential applications of such sensors is extremely wide: from dangerous gases detection to determining of food freshness. Monolayer organic field-effect transistors (OFETs) with additional receptor layer could be a perspective solution of this problem¹.

The proposed approach is to use a monolayer OFET-based sensor (Fig.1a) having semiconducting and receptor monolayers fabricated one on top the other by Langmuir-Schaefer (LS) technique. It combines high sensitivity provided by ultralow (a few nm) thickness of the active layer with high selectivity provided by the receptor layer.

Tetramethyldisiloxane dimers of dialkyl benzothieno[3,2-b][1]bithiophene (**BTBT**) derivatives with various aliphatic spacers and hexyl side groups were used as monolayer semiconductors in LS OFETs². Various porphyrin derivatives were used as the receptor layers capable of selective interaction with different target gases. It was established that additional receptor layer doesn't disturb the LS OFET performance. At the same time it was shown that OFET electrical characteristics (threshold voltage, source-drain current, on-off ratio) change if the target gases are present in the air even in trace amounts. Figure 1b represents an example of LS OFET sensor response to 5-10 ppm of ammonia at different relative humidity.

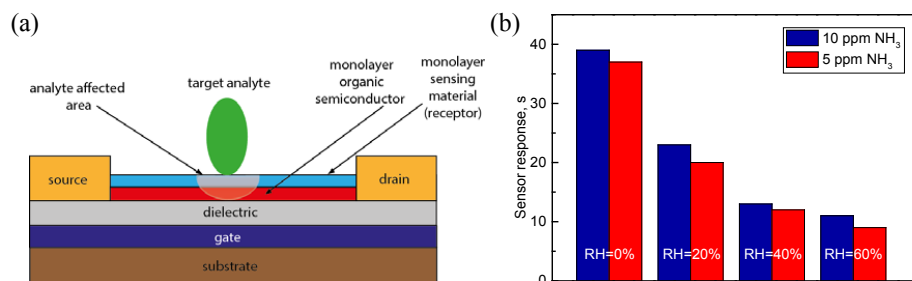


Fig. 1. Schematic representation of gas sensor based on monolayer LS OFET (a); sensor response to ammonia at different relative humidity (b).

As a result, gas sensors for ammonia and hydrogen sulfide based on LS OFETs with high sensitivity (lower than 5 ppm) to the target gases have been fabricated. Their competitive advantages compared to commercial analogues are potentially low cost, ambient working conditions, fast response and long lifetime of the sensor. High selectivity to water (more than 10³) of the gas sensors developed has been demonstrated.

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Chromophore-Containing Non-Linearly Optically Active and Light-Emitting Polymers

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Non-linear optical (NLO) nanostructured materials are of great interest for optoelectronics because they make it possible to change the frequency of the propagating light and to realize a communication between electric and optical signals through their light-perturbed electronic distribution. In the present work, thermally stable and heat resistant polyimides with covalently attached chromophore groups were synthesized by Mitsunobu reactions between OH- or COOH-functionalized polyimide and OH-containing chromophores. Some of the used azo-chromophores contained carbazole fragments to enhance polymer photoconductivity properties, which is necessary to create photorefractive holographic polymer media, or bulky side groups, preventing an undesirable centrosymmetric aggregation of chromophore groups. Second harmonic generation (SHG) coefficients, d_{33} , for corona-poled films of these polymers were measured. Films with the thickness of 0.1-2.0 μm were spin-cast on glass substrates from polymer solutions in cyclohexanone. Corona-poling was performed for 40-60 min at 150-200°C (depending on glass transition temperature of a particular chromophore-containing polymer). Rather high d_{33} values (>50 pm/V) were achieved.

For some azo-chromophore containing polyimides, the refractive index dispersion and frequency dependences of d_{33} values were measured in the fundamental frequency range from 800 to 1400 nm. All studied samples possessed a rather high beam resistance at the fundamental wavelength, their nonlinear optical properties remaining unchanged after the action of more than 10^4 pulses. It was shown that the frequency dependence of d_{33} is red-shifted with respect to the absorption spectrum. Therefore, there is a frequency range where the polymer is practically transparent, while the d_{33} values are still rather high.

Scientific and technological interest to conjugated polyfluorenes is due to their potential applications in optoelectronic devices, such as OLEDs, with the possibility to tune optical and electrical properties of the devices by varying the chemical structure of the polymers.

Suzuki and Yamamoto polycondensation reactions were used to synthesize new copolyfluorenes modified with 2,1,3-benzothiadiazole and Nile red luminophore units incorporated into the backbone and side chains, respectively, and various charge-transporting groups introduced into side chains. As a result of the optimization of the structure of copolyfluorenes, several novel copolymers were prepared with very efficient blue, green, red, and white electroluminescence, making these copolymers prospective for the design of such optoelectronic devices as full-color displays, energy-saving lighting devices, etc.

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Harnessing Molecular Diffusion in Organic Solar cell

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A main advantage in organic electronics is the solution casting processing. However, the rapid solution evaporation often leads to non-equilibrium morphology states. The metastable state means that significant morphology changes, mainly of the disordered regions, can occur spontaneously during the device fabrication and/or operation. Because the device performances are strictly correlated with film morphology, this “soft” characteristic often limits device performance and stability. Here we will show that the dynamic behavior of the film morphology can be judiciously harnessed to enhance device performances and stability. More specifically, we use the tendency of molecules to diffuse/migrate through selected domains in the film to study and direct desired morphologies and interactions in organic solar cells (OSC). This approach is demonstrated in two systems. In the first case, the spontaneous migration of selected additive molecules from within the active layer to form interlayers at the organic/metal interface¹. Using a plethora of techniques, we show that metal-additive interactions drive additive segregation to the organic/metal interface and that selected interlayers can significantly enhance Voc, FF and device efficiency². In a second example, selected gas-phase metal organic molecules diffuse into pre-formed OSC films to directly map film morphology^{3,4}. By following the diffusion patterns in P3HT and different fullerenes, we can spatially map the different P3HT:fullerene bulk heterojunctions and correlate HRSEM and HRTEM images of the nano-scale morphology with device performance.

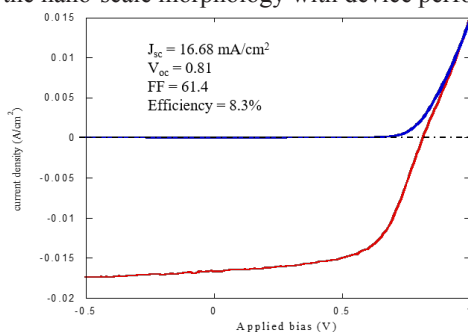


Fig. 1. J-V curves in dark and under illumination of small molecule OSC with spontaneously generated interlayer

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The Dynamics of Charge Separation in Organic Photovoltaic Materials with Low Electronic Band Offsets

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Numerous studies have shown that the open-circuit voltage in organic photovoltaic devices is determined by the energy of charge transfer (CT) states at the donor-acceptor interface, as well as the type of recombination. For this reason, recently major efforts have been directed towards reducing relaxation losses by minimizing the LUMO-LUMO offset between the donor and acceptor materials. However, this offset also determines the driving energy for charge separation and was shown to be critical for material photophysics (fig.1).

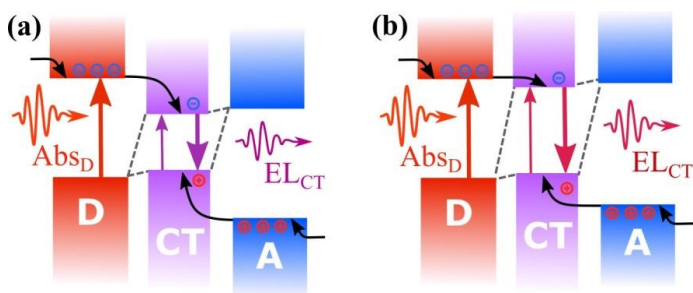


Fig. 1. The energy alignment and electronic dynamics in OPV materials with large (a) and small (b) driving energy for charge separation.

In this contribution, we summaries our recent findings on charge generation mechanism in organic donor:acceptor blends where driving energy is comparable or less than 0.1 eV. We use a combination of steady state techniques, like absorption and electroluminescence spectroscopy, to elucidate the energetics of CT states and ultrafast methods, like transient absorption and time-resolve photoluminescence, to reveal the charge dynamics. We show, that charge generation mechanism in these systems may be substantially different from previously studied large-driving-energy polymer:fullerene systems. For example, structural reorganisation may play substantial role in charge separation and recombination process leading to Marcus-type behavior in normal and inversed regimes.

This work was supported by Royal Society through University Research Fellowship and by China Scholarship Council.

Fullerene-free organic solar cells exceeding 1V open circuit voltages

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Optimizing the energy levels at the donor-acceptor interface of organic solar cells has driven their efficiencies to above 10%. However, further improvements towards efficiencies of typical for the best inorganic solar cells are difficult because of empirical limits for the open-circuit voltage of polymer fullerene solar cells which hardly ever exceeds 1V due to voltage loss >0.6 eV (Figure 1). Here we show that this limit is overcome with a non-fullerene acceptor where a rhodanine flanked non fullerene small molecule acceptor **FBR** serves as acceptor with and a low band gap polymer **PfBT4T-2DT** as donor material. The combination of **FBR** and **PfBT4T-2DT** allows both a high open-circuit voltage of 1.12V and extremely low voltage loss ~ 0.47 V whilst keeping the external quantum efficiencies $>55\%$ which could not be achieved with fullerene solar cells so far. These unconventional features result in photovoltaic performances as high as 7.8%. This study will inspire organic-photovoltaic community to focus on non-fullerene acceptors for further improvement of power conversion efficiencies without any complex multi-layer or -component device architectures.

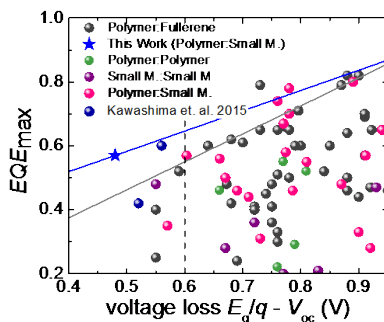


Figure 1. Comparison of the maximum external quantum efficiency and the voltage loss between E_g/q and the open circuit voltage V_{oc} for different types of organic solar cells. The grey line indicates the empirical limit for the maximum EQE_{max} possible for a given voltage loss given by Li et al.(REF) The blue line is determined using the result in the current work. Traditionally, there are hardly any cases of $EQE_{max} > 0.5$ with a voltage loss < 0.6 V. Novel results presented here as well as the results from Kawashima et al. show that it is possible to overcome this barrier.

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Device Structure Engineering for Organic and Hybrid Photovoltaics

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The advantages of Solution Processed molecular and hybrid Photovoltaics, such as their light weight, mechanical flexibility in addition to the small energy demand, and low cost equipment requirements for roll-to-roll printing mass production, characterize them as a dominant candidate source for future electrical power¹. The Presentation aims in covering a range of engineering issues needed to bring printed (organic and perovskite) solar cells^{2,3} to commercial viability in terms of efficiency⁴, lifetime⁵ and cost⁶. A systematic understanding of the relationship between electrodes, processing and device performance relevant to printed photovoltaics product development targets will be presented.

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Solution-processed organic tandem solar cells: interface design, process optimization and loss analysis

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The tandem concept is especially attractive for the organic photovoltaics (OPV) technologies owing to its potential to improve the power conversion efficiency (PCE) of single OPV cells by ~40%.¹ The construction of organic tandem solar cells is directly determined by the functionality and reliability of interfacial layers. The energy barriers between electrodes and absorbing layers have to be minimized by employing effective interfacial layers. The free charge carriers selectively extracted by the interfacial layers have to be conducted to the corresponding electrodes or to the intermediate layer with minimized losses. However, the commonly used p-type interfacial layer, PEDOT:PSS, does not perform well when coated on top of most high-performance organic donors, thus restricting their application in solution-processed organic tandem solar cells.

In this contribution, we will demonstrate interface design rules for solution-processed organic tandem solar cells. The interfacial layers developed by engineering are fully compatible with state-of-the-art organic donors, exhibiting great potential for realizing high-performance, solution-processed organic tandem solar cells.^{2,3,4,5} Moreover, a series of high-performance donors are investigated and analysed to tap their performance potential when processed in air by using a roll-to-roll compatible deposition method. Organic tandem solar cells with all the semiconducting layers printed in air achieve high PCEs over 10% along with unprecedented high fill factors >76%.

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**Exciton and charge separation dynamics in intermixed polymer:fullerene blends:
correlating structural and photophysical length scales**

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Photocurrent of bulk-heterojunction organic solar cells depends on the structure of the photoactive layer, in which molecularly-mixed and pure phases with different densities and sizes co-exist. The impact of these structures on the charge separation dynamics is however not well understood. In this work, we address this issue by studying the amorphous copolymers SiIDT-2FBT, SiIDT-DTBT and PCDTBT in blends with the fullerene PC70BM. By changing the blend composition, we modulate the size and concentration of the pure and intermixed domains on the nanometre length scale. Using time-resolved laser spectroscopy in combination with photoluminescence and electroluminescence experiments, we show that the changes in morphology correlate quantitatively with the changes in charge separation/recombination dynamics, and with changes of the charge transfer state emission. Photoexcitation of films with only a single molecularly-intermixed phase results in relatively strong photoluminescence from the charge transfer states and inefficient charge photogeneration limited by geminate recombination on the ns timescale. From intensity dependent studies, we determine the radius of the geminately recombining polaron pairs to be 3-5 nm. This is bigger than the size of the intermixed domains (1-3 nm) in the films with excess fullerene, where pure fullerene phases of <4 nm are formed. In the films with excess fullerene, photoluminescence from the charge transfer state diminishes and the nanosecond polaron geminate recombination channel is suppressed, by making the fullerene domains accessible for electron escape. The spectroscopy results are shown to correlate with device performance.

This work is part-funded by the European regional Development Fund through the Welsh Government, EPSRC (EP/IO1927B/1 and EP/K011987/1) and the National Research Fund of Luxembourg.

Interfacial electronic properties of air-stable molecule-doped polymers and fullerene derivatives for organic photovoltaics

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Understanding the interfacial properties is a key issue to improve the performance of organic electronics. As most organic devices were fabricated in a glove box with inert atmosphere by e.g. spin-coating. The interaction between these organic materials and their electrodes will fall in a region as weakly interacting series compared to the atomic clean surface in ultra-high vacuum. Such weakly interacting interface properties can be predicted by integer charge transfer model (ICT)¹, where the Fermi level is either pinned to negative/positive interface polarons or vacuum level alignment holds. The pinning behavior is due to spontaneous charge transfer across the interface via tunneling (integer charge transfer) when the substrate work function is higher (lower) than the energy required to oxidize (gained from reducing) a molecule at the interface.

Engineering the interface properties of the organic device in a controlled manner is another key issue to enhance the device performance. Doping has been proved as a powerful method to tailor the device performance compared to the pristine state, e.g. increasing the conductivity and mobility, decreasing the injection barrier as well as effectively suppressing geminate charge recombination at donor-acceptor interface via filling of the so-called tail states^{2,3}. The influence of doping upon interface energetics is critical for understanding the process so as to enhance power efficiency conversion. However, how the doping influences the energy level alignment between organic materials/electrode is still an open question.

Here we will explore the energetics of the molecule-doped conjugated donor polymer and acceptor fullerenes/electrode interface in solution processing to span the range of low-intermediate-high doping concentration. For the donor polymers, we selected rr-P3HT (crystalline), TQ1 (amorphous) for comparison order and disorder system upon doping, where F4TCNQ molecule was chosen as p-type dopant⁴. Benefit from the recently developed air-stable n-type dopant N-DMBI³, the solution doped fullerene (C₆₀) and their derivatives (PC₆₀BM, ICBA) becomes possible, as well as non-fullerene acceptor⁵. We will conclusively establish its universal energy level alignment holding for all doped organic semiconductor systems, in which ICT model still work with additional dipole shift needed. We also highlight different doping behaviors upon the n-type and p-type dopants, and the molecular length regarding their interface energetic properties.

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Controlling the recombination in ternary polymer blends: a path towards high efficiency organic photovoltaics

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One key advantage of solution-processable organic semiconductors is the opportunity of blending different materials in order to attain novel material properties and applications. The concept of ternary blend organic solar cells makes use of exactly that idea: three (or more) organic chromophores are combined to better match the solar irradiance spectrum and thus increase the amount of light absorbed, which in turn will increase the power output of the solar cell¹. However, charge transport limitations of many current generation polymer blends typically require rather low active layer thicknesses (around 100 nm) for optimum performance². Here, we design two advanced material composites leading to a high fill factor in ternary blends, thus demonstrating how the recombination thresholds can be overcome³. Moreover, we successfully demonstrate devices with unusually thick active layer (>300 nm) and power conversion efficiency beyond 11%⁴. Motivated by the possibility to process thick-film devices based on ternary blends, we demonstrate solar modules consisting of three in series connected solar cells, delivering 8.2% and 6.8% power conversion efficiency on glass and flexible substrates, respectively. These results underscore the relevance of ternary photovoltaic polymer blends for future upscaling technologies.

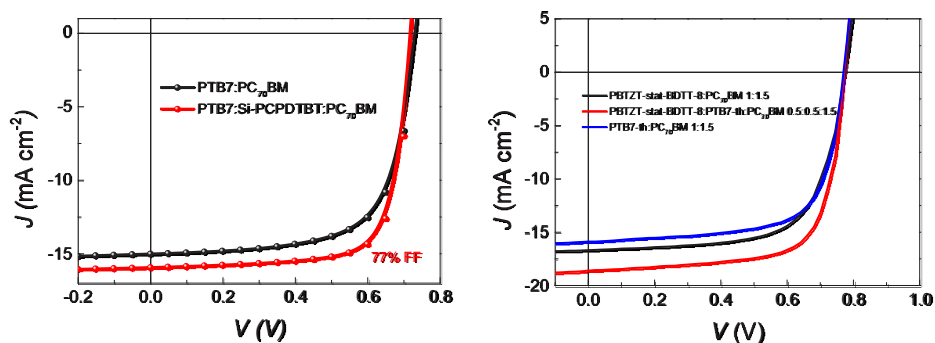


Figure 1. J-V characteristics of binary and ternary BHJ solar cells under solar simulator illumination (100 mW cm^{-2}).

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Poster presentations

Intrinsic Thermal and Photochemical Stability of Hybrid and Inorganic Lead Halide Based Perovskites

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Here we will discuss thermal and photochemical degradation pathways of a series of complex haloplumbates APbX_3 ($\text{X}=\text{I}, \text{Br}$) with organic ($\text{A}^+=\text{CH}_3\text{NH}_3^+$, $[\text{HC}(\text{NH}_2)_2]^+$) and inorganic ($\text{A}^+=\text{Cs}^+$) cations in the absence of exposure to oxygen and moisture (glove box environment). It has been shown that the most common hybrid materials (e.g. MAPbI_3) undergo strong thermal degradation at the temperatures of $\sim 80\text{-}90^\circ\text{C}$. Light-induced degradation of the same materials occurs rapidly at $40\text{-}50^\circ\text{C}$ and cannot be completely prevented even while cooling the samples down to $10\text{-}15^\circ\text{C}$. It has been revealed that thermal and photochemical aging of MAPbI_3 proceed *via* different chemical pathways and produce different products.

The obtained results strongly suggest that intensively investigated hybrid lead halide based perovskites are intrinsically unstable under the realistic solar cells operation conditions and their practical implementation might be very challenging. On the contrary, the cesium-based all inorganic complex lead halides revealed far superior stability and, therefore, provide an impetus for creation of highly efficient and stable perovskite solar cells that can potentially achieve pragmatic operational benchmarks.

Towards designing new high-mobility polymeric semiconductors: DFT Investigation of electronic and optical properties of BTI-based monomers and dimers

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Designing of new high-mobility polymeric semiconductors to be usable in the organic field effective transistor (OFET) devices with good processability and environmental stability is still a challenge. In this study, we focused on the bithiophene-imide (BTI)^{1,2} (Fig.1) based organic molecules which were modeled by combining the BTI unit with different aromatic benzene or thiophene rings. The obtained comonomers and also their dimers were subjected to geometry optimizations by using the Density Functional Theory (DFT) method at B3LYP/6-311+g(d,p) level of the theory. The effect of the R1 groups and the chain length of the backbone on the electronic properties such as electrostatic charge distributions, HOMO and LUMO energies and band gaps were investigated.

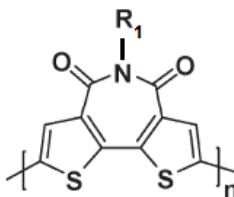


Fig. 1. Bitiyoferimide (BTI) monomer unit (R1: H, NO₂, NH₂, OH, F, Cl, Br, I).

Time dependent DFT (TD-DFT) method at same level of the theory was used to calculate the energies of the excited states and the UV-VIS frequencies corresponding to the electronic transitions were determined. UV-VIS spectra of all derivatives of the comonomers and the dimers were analyzed in terms of the spectral shifts due to the impact of R1 substitution and lengthening of the chains. The studies on the molecules at the monomeric and dimeric states are the preliminary studies which will then be extended to polymers, to evaluate eligibilities of modeled polymeric films for OFET devices.

This work was supported by TUBITAK (project № 115Z501).

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Non-volatile Memory Devices Based on Ferroelectric Polymer and Semiconducting Silicon

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Non-volatile memory devices based on simple 2-terminal ferroelectric diodes are being extensively investigated as viable logic components in low-cost and printable electronics. There are various reports on all-organic ferroelectric diodes that will gradually pave the way towards successful implementation of memory cells on a plastic roll^{1,2,3,4}. However, the mechanism of resistive switching, influenced by material morphology as well as the interplay between the ferroelectric, semiconducting, and metal interfaces, is still not fully understood. In this study, we investigate the influence of ferroelectric polarization of poly(vinylidene fluoride-co-trifluoroethylene) P(VDF-TrFE) on charge modulation of semiconducting Silicon by fabricating hybrid devices depicted in Figure 1. Electrical characterization is used to evaluate the performance of the diodes.

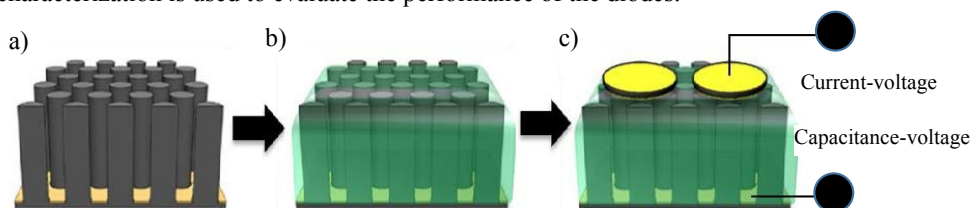


Fig. 1. Schematic of memory device fabrication. a) fabricate nSi nanopillars followed by b) solution casting of ferroelectric polymer (green) and finally c) evaporating top contacts to monitor characteristics of resistive switching⁵.

This work was supported by the Natural Sciences and Engineering Research Council (NSERC) and the Alberta/Technical University of Munich International Graduate School for Hybrid Functional Materials (ATUMS).

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Effect of evaporated and laminated gold electrodes on performance of organic single crystal field effect transistors

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Ambipolar organic field-effect transistors (OFETs) based on single-crystals attract many researchers as they can lead to efficient light-emitting devices (LEFETs) with higher emission efficiencies compared to the organic light emitting diodes¹. Among various types of ambipolar OFETs, single-crystal bottom-gate top-contact devices based on thiophene-phenylene co-oligomers (TPCOs) show the best performance combining efficient charge transport and high luminescence quantum yield [2]. However, the LEFET energy efficiency is still very low. One of the biggest challenges for high performance single-crystal ambipolar OFETs is to overcome their high threshold voltages, which can be associated with high contact resistance. New approaches for deposition of ohmic contacts with low contact resistance have to be developed.

In this work, we compare evaporated and laminated gold electrodes on top of the thiophene/phenylene (TMS-PTTP-TMS) and furan/phenylene (BPFB) co-oligomer single crystals grown using physical vapor transport (PVT) technique^{2,3}. OFETs based on this crystal were fabricated in the bottom-gate top-contact geometry (Figure 1) and their performance was compared. Figure 1 presents transfer characteristics of OFETs with laminated and evaporated electrodes. Laminated gold contacts resulted in the reduced threshold voltage down to 0 V compared to the devices with evaporated gold electrodes. We analyze ambipolar OFETs with asymmetrical top contacts: an electron-injecting electrode formed by evaporation of low work function metals (Ca, Al) and a hole-injecting laminated gold electrode. Thus, the laminated gold electrodes resulted in ohmic contact providing zero threshold voltages and are promising for efficient single-crystal OFETs.

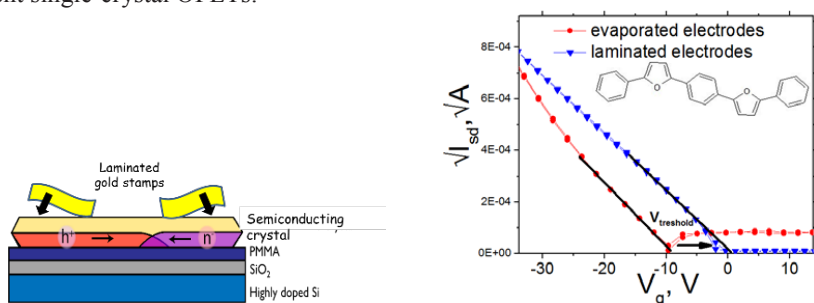


Fig. 1 Device geometry (left) and transfer characteristic of OFETs based on BPFB crystal with laminated and evaporated gold electrodes (right)

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

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Shellac film as gate insulating layers in organic field-effect transistors

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So far, organic electronics technology has been developed focusing on low-cost, solution-processed, and mechanically flexible characteristics. According to the very recent reports, these merits allow the organic electronics to expand their applications to biomedical devices that can be stuck onto (or even implanted in) a human body.¹ However, additional material properties such as bio-compatibility or bio-degradability must be considered in order to be used for fabrication of the organic bioelectronic devices. Shellac, a natural resin secreted by the female lac bug on trees, is regarded as a promising material for organic bioelectronic devices due to its safety and innocuousness for human body. Indeed, shellac has been widely used as a brush-on colorant such as nail paint, wood finish for string instruments and food glaze. In addition, it was also used in electrical applications because it has good electrical insulating property and seals out moisture.

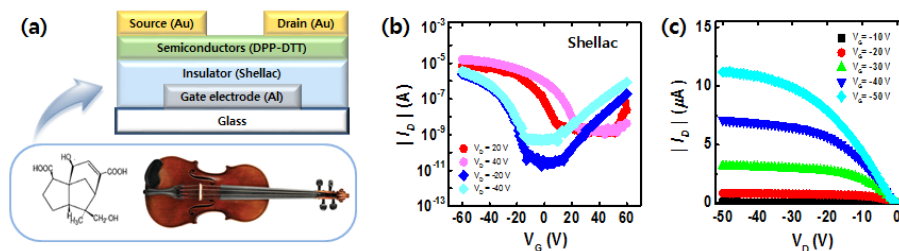


Fig. 1. (a) Device structure, chemical structure of Shellac, widely used natural varnish resin for string instrument. (b) Transfer curves and (c) output curves of OFETs with shellac dielectric layers.

In this presentation, we will introduce the feasibility of the shellac as a gate dielectric material in organic field-effect transistors (OFETs), critical switching components in organic biomedical electronics. Fig. 1(a) shows a schematic inverted staggered structure of the OFET we fabricated and chemical structure of the shellac. For the fabrication of the OFET, we have used DPP-based polymer semiconductor (diketopyrrolo-pyrrole-dithiophene-thienothiophene, DPP-DTT) for active channel and Au and Al were used as source/drain electrode and gate electrode, respectively. Fig. 1(b) and (c) exhibit the transfer and output curves of the fabricated OFETs with shellac dielectric layer. As shown in the electrical characteristic curves, the DPP polymer semiconductor based OFETs with the shellac dielectrics were properly operated showing the ambipolar characteristics with the field-effect mobility of 0.064 cm²/vs and 0.044 cm²/vs for hole and electron, respectively. From our preliminary results of the DPP-DTT based OFETs with the shellac dielectric, it is suggested that the use of the shellac as a dielectric layer is promising for the fabrication of organic bioelectronics devices.

This work was supported by the Basic Science Research Program through the National Research Foundation (NRF) funded by the Ministry of Science, ICT, and Future Planning of Korea (Code No. 2015R1C1A1A02037534).

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Star-shaped donor-acceptor oligomer with p-fluorophenyldicyanovinyl electron-withdrawing groups for organic photovoltaics

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Obtaining stable organic semiconductors based on ordered bulk-heterojunction is one of the recent organic photovoltaics problem. A novel type of p-type organic semiconductors based on star-shaped oligomers able to self-organize into ordered columnar phase recently been developed in our laboratory ¹⁻⁴. In this work new star-shaped oligothiophenes containing p-fluorophenyl dicyanovinyl electron-withdrawing groups, linked through bithiophene π -spacer with electron-donating either triphenylamine core were synthesized (Figure 1). The electrochemical, thermal and optical properties of this compound were investigated by cyclic voltammetry, differential scanning calorimetry, thermogravimetric analysis and UV-Vis spectroscopy with interesting optical and thermal properties exhibition. This compound was applied as donor material in solution processable bulk heterojunction organic photovoltaic devices.

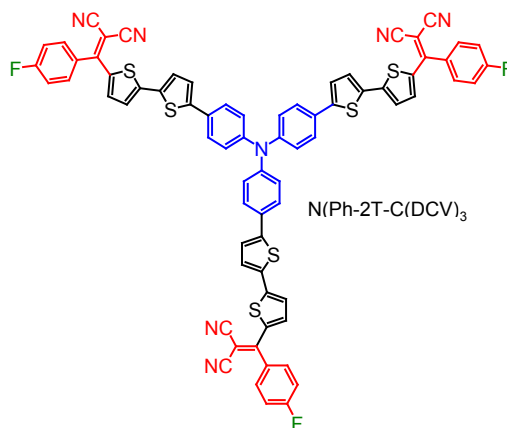


Fig. 1. Schematic structure of star-shaped D-A oligomer with p-fluorophenyl substituents
This work was supported by Russian Scientific Foundation (project № 14-13-01380).

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Synthesis of substituted diaza-analogues of pyrene and perylene

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Heterocyclic analogues of perylene and pyrene are of interest for organic electronics but are poorly understood. Number of such compounds known to date is small and the methods for their synthesis are few.¹

We developed novel approach to the synthesis of substituted diazaperylenes and diazabenzopyrenes which bases on heterocyclization of bis(R-ethynyl)anthraquinones with urea.² Construction of the pentacyclic core was realized on annulation of the two pyridine rings to the anthraquinone skeleton. Note that this synthetic approach is quite simple and does not require organometallic compounds or aggressive conditions.

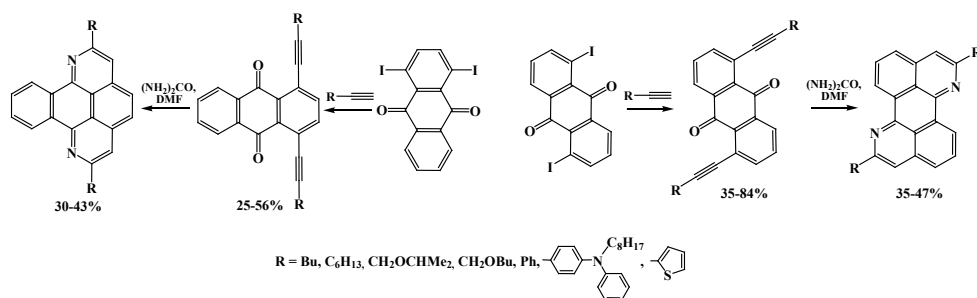


Fig. 1. Scheme of synthesis of diazabenzopyrenes and diazaperylenes

The method which demonstrated broad synthetic capabilities was tested in the preparation of polycondensed molecules with substituents of different types (aliphatic, aromatic, heteroaromatic). Thereby there are opportunities to change properties of the products. For example, the strongest effect was revealed for compounds containing diphenylamine substituents: decreasing of HOMO-LUMO gaps and luminescence yields, and increasing of extinction coefficients were observed. Synthesized diazabenzopyrenes and diazaperylenes are convenient building blocks, which can be used in the synthesis of the new small molecules, oligomers and copolymers.

This work was supported by RFBR (project № 16-03-00082a).

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Analytical theory for charge carrier recombination in blend organic solar cells

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The apparent order δ of non-geminate recombination higher than $\delta = 2$ has been evidenced in numerous experiments on organic bulk heterojunction (BHJ) structures intensively studied for photovoltaic applications¹. This feature is claimed puzzling, since the rate of the bimolecular recombination in organic BHJ systems is proportional to the product of the concentrations of recombining electrons and holes and therefore the reaction order $\delta = 2$ is expected.

In organic BHJ structures, electrons and holes are confined to two different material phases: electrons to the acceptor material (usually a fullerene derivative) while holes to the donor phase (usually a polymer). The non-geminate recombination of charge carriers can therefore happen only at the interfaces between the two phases. Considering a simple geometrical model of the BHJ system, it has been recently shown that the apparent order of recombination can deviate from $\delta = 2$ due solely to the topological structure of the system².

In the current report, we show, using analytical theory that the geometry of the recombination problem leads to the deviation of the carrier concentration in the vicinity of the interface from the average concentration in the bulk. Conditions are considered, at which this difference can lead to the deviations of the apparent recombination order from the value $\delta = 2$ that is generally expected for bimolecular reactions. The theory is universal in the sense that it is based solely on the inhomogeneous distributions of the recombining species.

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Hybrid Organic/Inorganic Interfaces as Reversible Label-free Platform for Sensing and Biosensing

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The combination of organic and inorganic materials to create hybrid functional nanostructures can be considered an effective approach to develop label-free sensors and biosensors. Hybrid oxide/molecule nanostructures have already been widely exploited in different electronic applications¹. On sensors, additional advantages may be achieved by making use of solid-liquid interfaces for the detection of specific analytes. Insulator/electrolyte interfaces, for instance, have been widely exploited on transistor-like structures for detecting/monitoring organic solvents². In this work, we combine an ultra-thin high-k dielectric layer with a nanostructured organic tail to create a platform capable of direct monitoring biospecific interactions and specific molecules at the electrode's surface. The devices can be compacted by using rollup strained nanomembranes³. The sensor's architecture and operation relies on the functionalization of 3.3 nm Al₂O₃ with a functional bioactive tail⁴. Such structure allows the measurement of the net charge variations at the solid (hybrid) - liquid interface. The device electrical characterization was performed in aqueous solution by means of impedance spectroscopy. The Al₂O₃ dielectric constant was obtained as well as a protocol to stabilize the oxide in aqueous solution established. In order to demonstrate the operation device as an analytical tool, a sensor to determine the concentration of water in ethanol solution was developed⁵. This application is of interest for fuel qualification. In addition, by incorporating a bifunctional tail, a reversible and compact label-free glutathione-S-transferase (GST) biosensor is demonstrated. The biosensor shows a linear range of operation from 200 pmol.L⁻¹ to 2 μmol.L⁻¹, the largest range reported in the literature for GST label-free sensors.⁴ By combining specific aptamers on the oxide layer, we were able to monitor the presence of toxins in water.

SIBRATEC-Nano and FAPESP (Project 2014/25979-2) are acknowledged.

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Stimuli responsive emissive behaviours of organic and organometallic compounds with crystallization induced emission properties

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While most of the luminogens undergo a reduction of the emission properties upon aggregation, some compounds, while non-emissive in solution, become emissive in the solid state. These phenomena are often described as Aggregation Induced Emission (AIE). Since most of the applications in optical and optoelectronic devices require solid state materials, the interest in compounds showing AIE has been receiving increasing attentions. Recently Aggregation-Induced Phosphorescence (AIP) was reported for some Iridium(III) complexes and the search for other organometallic compounds showing this property has become particularly relevant for OLED technology.

In some materials the enhancement of the emission efficiency occurs only if aggregation induces a proper crystal packing and not in the amorphous phase. The aggregation conditions in these so called Crystallization Induced Emission (CIE) systems are strictly related to the particular molecular structure of the luminogens. In this work some examples of such materials will be discussed in order to shed light into their photoexcitation properties.

The comparison of different crystal polymorphs of a simple push-pull organic molecule¹, of Bismuth^{2,3,4,5} and Lead⁶ complexes and coordination polymers evidences the important role of the crystal packing in both fluorescent and phosphorescent luminogens that show CIE. In the discussed examples, even weak intermolecular interactions do affect the photophysical properties of materials whose emission is originated by restriction of intramolecular motions. For these reasons such materials display stimuli responsive (mechanochromic and thermochromic)^{5,6} emissive behaviour that could be exploited in the construction of pressure and thermal sensors.

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Investigation of hybrid organic / inorganic heterostructures in GaN for light emission

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GaN nanowires (NW) with different doping domains have become a promising candidate for efficient blue LEDs. The application in white light LEDs though has the problem known as the green-gap that may be solved by utilizing a hybrid organic / inorganic approach. In this study we investigate the properties of the type II interface between the GaN and organic emitters, as it has been previously done for ZnO¹. For this purpose TRPL is employed using m-plane GaN as a model system for the NW sides which exhibit similar m-plane facets. The effect will be further studied with a series of different types of organic emitters such as singlet versus triplet emitters.

This work was supported by BMBF (project № FKZ 13N10724).

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Vertical Cavity Laser on Thiophene-Phenylene Co Oligomers

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Recent development of novel organic crystalline semiconducting materials that combine both high luminescence and charge transport properties opens a route to new types of optoelectronic devices. One of the most aspired of them is injection organic laser, and organic single-crystal light emitting transistor (OLET) is considered to be one of the most promising platforms for lasing. Among various organic semiconducting materials for organic lasers, thiophene-phenylene co-oligomers (TPCO) single crystals are one of the top candidates.

The use of vertical cavity with crystalline semiconducting organic materials could significantly reduce the lasing threshold comparing to conventional methods such as using the organic crystal as a waveguide. In this work, we study a vertical cavity laser with a promising thiophene-phenylene co-oligomer (TPCO), TMS-PTPTP-TMS (Fig. a). To understand lasing properties of the material, lasing was investigated in solid TMS-PTPTP-TMS solution in poly(methyl methacrylate) (PMMA). Fig. d shows the schematic of the laser built using plane mirrors.

Lasing was demonstrated with a 355-nm 10-ns pumping laser (Fig. a, b, c). The emission wavelength of the laser is 460 nm. The good features of vertical cavity laser are that it has single spectral band and the PL is not visible unlike usual amplified spontaneous emission (ASE) behavior of typical crystalline laser. The average laser generation threshold was estimated as 2.4 uJ. We suggest that the threshold can be significantly lowered by using higher quality cavity at the given wavelength.

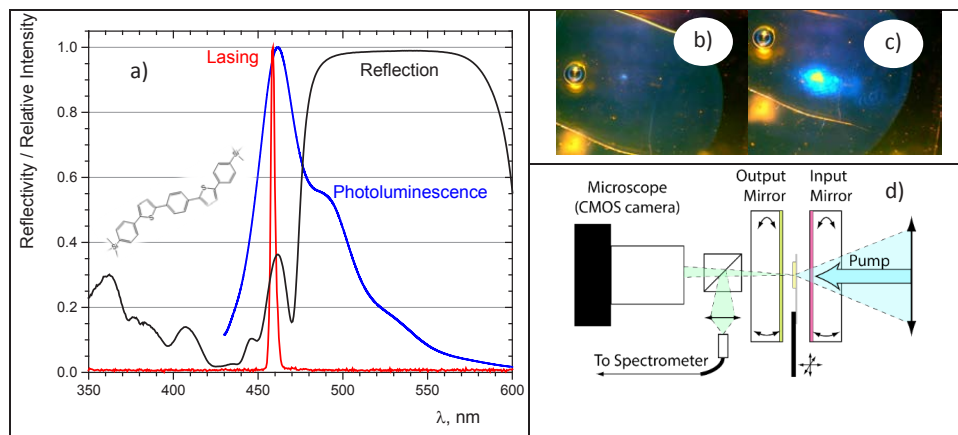


Fig. Laser emission, PL and cavity reflection spectra and chemical structure (a); microscope pictures showing PL (b), and lasing (c); cavity configuration (d).

The results presented in this work allow us to expect the possibility to significantly decrease the lasing threshold compared to the crystalline waveguided cavity by introducing an external high Q-factor vertical cavity.

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

Metal-containing porphyrins as an active layers for organic field-effect transistors and gas sensors on their base.

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Metal-containing porphyrins and their derivatives are perspective functional materials for different applications in organic electronic: organic light-emitting diodes, organic solar cells¹, organic field-effect transistors (OFET) and gas sensors on their base².

In our work various porphyrins previously modified by palladium catalyzed C-H-activation were used as an active semiconducting or additional receptor layers in OFETs. Monolayer and bulk films were fabricated on the base of these porphyrins by Langmuir-Schaefer (LS) and spin-coating (SC) techniques. Morphology of the films was studied by polarizing optical and atomic force microscopies. It was found that the bulk films have thickness of ~15 nm, while monolayer films have thickness of ~2 nm. Film morphologies were quite different and depend on metal chemistry: from completely uniform layer of titanium oxide porphyrin (Fig. 1a) to «spiderweb» structure of ferric chloride porphyrin (Fig. 1b).

OFETs with bottom-gate and bottom gold electrodes were manufactured using porphyrin-based LS and SC films as semiconducting layers and only bulk films show semiconducting properties. Their electrical behavior was typical for p-type OFETs with a hole mobility of $\sim 10^{-6}$ cm²/Vs and threshold voltage was around -5V. The post-deposition solvent vapor annealing of the semiconducting layer resulted in re-crystallization of the layer with polycrystalline non-ordered structure formation that caused charge carrier mobility decreasing due to losses on the boundaries of separate crystallites. Usage of porphyrin-based LS monolayers as receptor layers of gas sensors was more successful and allowed fabrication of gas sensors for ammonia and hydrogen sulfide with high sensitivity (~5 ppm). Influence of porphyrin chemistry and layer thickness on sensor selectivity and sensitivity was investigated.

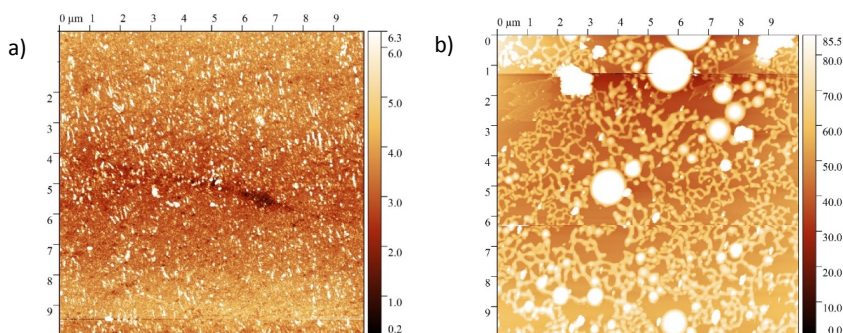


Fig.1 Morphology of LS films based on metal-containing porphyrins: TiO (a) and FeCl (b).

This work supported by RFBR (grant 17-03-00222).

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Active organic semiconductors based on 10,15-dihydro-5*H*-diindolo[3,2- α :3',2'-c]carbazole as a centre core for OTFTs

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Triindole (10,15-dihydro-5*H*-diindolo[3,2- α :3',2'-c]carbazole) is a very promising organic semiconductor for optoelectronic applications. In fact, some triindole derivatives have been reported already as suitable organic materials for OPVs¹, OLEDs² and, recently, in OTFTs³. The triindole core, a planar disk-like molecule with C³-symmetry, can be considered as an extended π -system where three carbazole heterocycles share an aromatic ring. Importantly, it presents three reactive N-H units that allow the easy introduction of alkyl chains, which not only increase the solubility of the system, but also can affect the molecular order within the semiconductive layer of the final electronic device. On the other hand, triindole can be symmetrically functionalized at the 3, 8 and 13 or at the 2, 7 and 12 positions enabling the extension of its π core.

With this in mind, we have been engaged in the synthesis and characterization of new triindole derivatives. It was considered the extension of the π -conjugated triindole system by introducing donor moieties. Specifically, the groups selected have been the phenyl, naphthyl, methylthienyl and benzothienyl placed at 3,8,13 positions of the triindole core (Fig. 1). Finally, their semiconductive properties have been analysed as organic active layer on OTFTs showing high stability under ambient conditions.

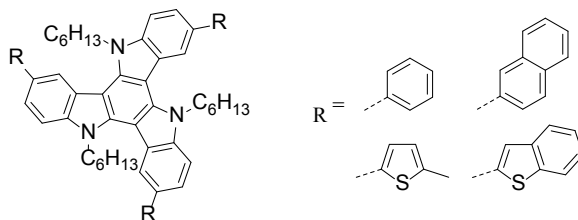


Fig. 1. General chemical structure of triindole derivatives.

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Molecular structure – electrical performance relationship for photochromic materials used in the OFET-based memory devices

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Memory devices based on organic field-effect transistors (OFETs) have been intensively explored within the last few years. Memory behavior has been realized using different types of charge-trapping materials, ferroelectric polymers and various electrets.¹ Optical memory elements based on light-switchable OFETs have also been reported.² Organic photochromic molecules, e.g. diarylethenes, represent molecular switches, which undergo reversible isomerization between two quasi-stable forms under illumination.³ Therefore, these compounds represent a promising family of materials for designing OFET-based optical memories.

Here we report a systematic study of a series of photochromic bis(hetaryl)ethenes bearing different functional groups R (Fig. 1) in photoswitchable transistors and memory elements. In particular, we analyzed programming speeds, width of the memory windows, write-read-erase cycling stability and retention characteristics of the devices. It has been shown that even minor differences in the chemical structures of photochromic materials can cause substantial changes in the electrical characteristics of the memory devices.

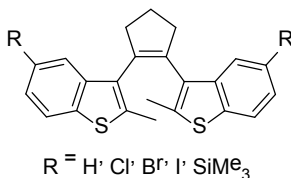


Fig. 1. Molecular structures of the investigated photochromic bis(hetaryl)ethenes

A thorough analysis of the obtained comprehensive set of the experimental data allowed us to establish some important correlations between the molecular structures of the materials and their electrical performance in memory elements.

This work was supported by RFBR (project № 15-03-06175).

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Synthesis and photophysical characterization of $Y_3N@C_{80}$ nitride clusterfullerene's derivatives

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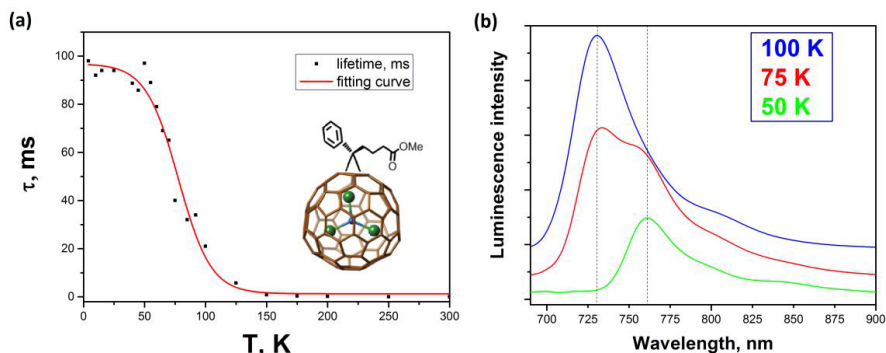


Fig. 1. (a) Luminescence lifetimes of $Y_3N@C_{80}$ PCBM derivative in polystyrene film at different temperatures; (b) luminescence spectra of $Y_3N@C_{80}$ PCBM derivative in frozen toluene solution at different temperatures.

Thermally activated delayed fluorescence (TADF) is a promising phenomenon for optoelectronic applications, such as in organic light-emitting diodes (OLEDs), and this topic has drawn research attention during the recent years¹. The significant feature of TADF molecules is their ability to harvest both singlet (S1) and triplet (T1) excited states in the form of efficient radiative emission, namely fluorescence. This is done by activating the reverse intersystem crossing (T1 → S1) process, which upgrades OLED performance significantly. $Y_3N@C_{80}$ is a type of nitride clusterfullerenes (NCFs)² family that exhibit emission mechanism due to a prompt and delayed fluorescence. Herein, we report the effect of $Y_3N@C_{80}$ derivatization with different functional groups on its emission process. Combination of continuous and time-resolved luminescence measurements at different conditions (absence of oxygen, temperature) revealed changes in the absorption and emission spectra. These changes might be assigned to the degree of fullerene's π -system perturbation, which depends on the functional group type and the attachment place. Therefore, our research provides first attempts to understand the impact of functionalization of $Y_3N@C_{80}$ NCF's carbon cage on the TADF effect³.

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Molecular end groups impact on structural and electronic properties of thiophene-phenylene co-oligomer single crystals

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⁶Academy of Labour and Social Relations

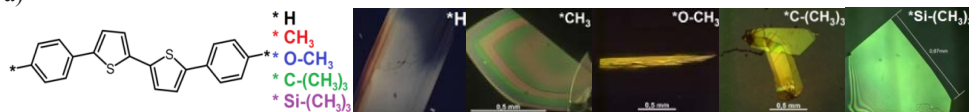
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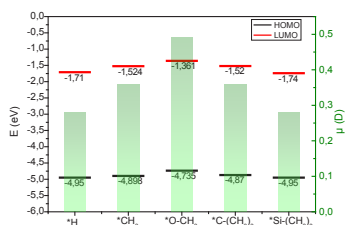
Single crystals of thiophene-phenylene co-oligomers (TPCO) are promising optoelectronic materials for light-emitting devices as they combine efficient charge carrier transport and high luminescence^{1,2}. These electronic properties are controlled by the chemical structure of the molecules and their crystal packing; however, the structure-property relationships in TPCO single crystals have not yet been properly understood.

Here, we study the impact of molecular end-groups on the structural and electronic properties of vapor-grown TPCO single crystals with the same phenylene-thiophene-thiophene-phenylene (PTTP) conjugated core (Fig. 1a, left) using optical/atomic force microscopy, x-ray diffraction, DFT calculations, contact angle measurements and field-effect transistor (FET) measurements.

a)



b)



c)

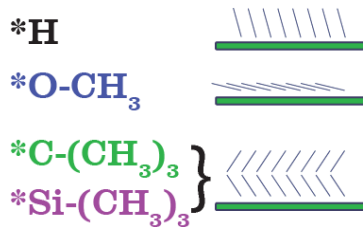


Fig. 1. a) Chemical structure of TPCO and microscopy images of crystals, b) HOMO/LUMO energies (DFT with 6-31g* basis set), c) molecule-substrate orientations in the single crystals.

Calculated HOMO and LUMO energy levels of the TPCOs (Fig.1b) show their small variation (<0.22 eV) with the end-group type; however, the static dipole moment of half TPCO varies noticeably. Variation of the end-group types results in a significant impact on the crystal shape (Fig. 1a), the molecular orientation vs their basal plane according to x-ray data (Fig. 1c), and the surface energy. Top-contact top-gate TPCO single-crystal FETs with printed electrodes exhibited p-type semiconductor behavior with charge carrier mobility in the range 0.03–0.1 cm²/Vs. We discuss the FET performance in relation with structural features of the TPCO single crystals.

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Modeling resistive switching: filamentary model and scaling limits for organic ReRAM

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The resistive switching effect (RS), an effect of reversible switching of material conductivity by few orders of magnitude due to applied electrical pulse, albeit being discovered in the 60s¹ is still a phenomenon that lacks fully and well accepted explanation for a lot of tested materials and devices' architecture². Organic resistive memory, as all organic technology, is considered cheaper and easier to manufacture than conventional inorganic devices, could be manufactured using biocompatible materials and this all with performance characteristic suitable for some specific types of application^{3,4}. In this work we present modeling of switching processes in ReRAM which is consistent with our experimental data for both large scale and printed organic composite devices.

The potential nonvolatile memory usage of resistive switching effect is, in its simplest form postulating "0" for high-resistance state (HRS), in which there are no conductive paths between device's contacts, and "1" for low-resistance state (LRS) in which filamentary conductivity is formed. Observable switching speed in both directions could be below 15ns with on/off ratio at least 2 orders of magnitude and higher than 10⁵ switching endurance⁴.

The main idea is the usage filament formation model, which is well described for inorganic devices in recent review by D. Ielmini⁵, and the idea that filament wall evolution could be described by Arrhenius law, i.e. activation-like dependency of filament radius⁶.

We have used our experimental data for polymer and polymer-metal composite devices, both large scale and based on ink-jet printed conductive patterns (minimal feature size 52μm). We have modeled devices behavior with account to experimentally present characteristics such as devices materials and their properties of thermal and electrical conductivity, devices dimensions, and experimental voltage sweep-rate. We found, that despite some models and experiments leading to result that winner-takes-it-all, i.e. the single conductive filament formation is the only situation possible⁷, for large enough devices both situations – formation and rupture of single dominating conductive filament and formation of multi-filament structures (which could occur after multiple switches due to accumulation of metal particles in polymer matrix and existence of multiple slightly dissolved filaments which then could be reformed simultaneously) are possible. In assuming of metal-based conductive filament we estimated the formed filament size in all cases to be below 50nm in diameter and full device (single bit) size that eliminates cross-talk phenomena to be below 1μm, which is on par with most recently developed printing techniques for conductive patterns⁸.

Overall, the results of the simulation well explain our observed data in accordance to filament formation model and highlight the path for future possibilities.

This work was supported by RFBR (project № 16-07-00961, 15-29-01267, 15-07-06081).

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The role of carbon lattice functionalization on transport properties in polyaniline molecular channel formed in gap between single-walled carbon nanotubes

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Individual molecules are the versatile tool for ultimately scaled electronic devices fabrication. Conjugated polymers are widely used to produce nanoscale diodes, field-effect transistors (FET), and sensor structures. The ends of nanotubes can drastically change the properties of molecular junction due to the different bondings between molecule and dangling carbon atoms. In this work, we investigate the influence of the side groups attached to carbon nanotubes on the conductivity and transport properties of polyaniline molecule junctions.

Two types of carbon nanotubes were used. Single-walled carbon nanotubes (SWCNTs) (provided by Professor A. Nasibulin, Skoltech) were deposited onto Si/SiO₂ substrate using gas-phase process formation based on thermal decomposition of ferrocene in the presence of carbon monoxide. Carboxylized SWCNTs (Sigma-Aldrich) were deposited onto Si/SiO₂ substrate using spin-coating technique. Source and drain Au/Ti electrodes (100/15 nm) were fabricated by photolithography, the gate electrode was high doped (p⁺⁺) Si substrate. Using focused ion beam we cut SWCNTs between 2 μ m gold contacts and made gaps of 30-40 nm. Polyaniline molecules were deposited from N-methyl-2-pyrrolidone solution into the gaps between SWCNTs using drop casting and electrophoresis methods. The morphological, optical and I-V characteristics of FET devices were measured at all stages of fabrication.

We produced FET devices based on 40 nm polyaniline molecular channel with linear mobility as high as 0.3 cm²/(V·s) for pristine SWCNTs and 21 cm²/(V·s) for functionalized SWCNTs contacts. Carboxylic groups increase the bonding between SWCNTs and polyaniline molecules through hydrogen bonds formation, which results in huge carrier injection from functionalized nanotubes compared to pristine SWCNTs and lower contact resistance. Easy preparation and good transport properties of polyaniline molecular devices with carbon nanotubes electrodes can be prospect and indispensable in polymer and single-molecule organic nanoelectronics.

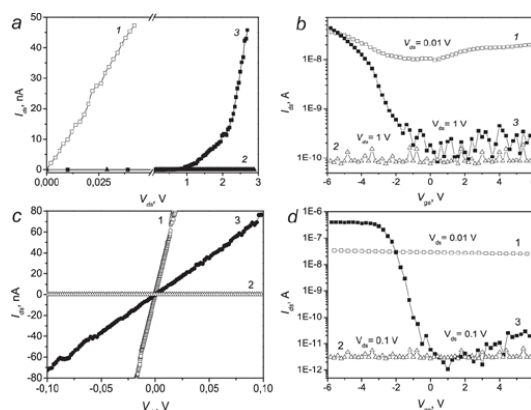


Figure 1. Output I-V curves for pristine (a) and functionalized (c) SWCNT. Transfer I-V curves for pristine (b) and functionalized (d) SWCNT. The numbers in all figures related to: 1 – before cut, 2 – after cut, 3 – after polyaniline deposition.

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Effect of electron acceptor groups on molecular properties of potential n-type semiconducting materials

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A series of naphthalene (**II**) and anthracene (**III**) -oligothienyl derivatives with electron acceptor groups (carbonyl-, cyano-, nitro-, etc.) as potential n-type semiconductors were designed and most of them were successfully synthesized (Fig.1). Here we present comparison of theoretical and experimental values of energy gap of these derivatives and influence of different electron acceptor groups (EWG) on electrochemical properties.

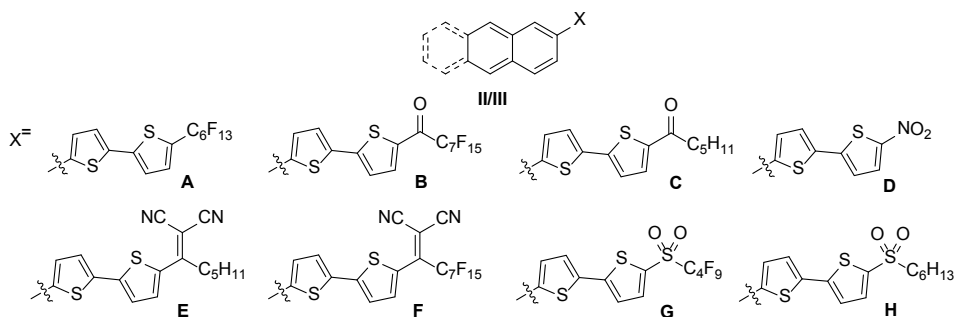


Figure 1 Designed structures with supposed n-type characteristics.

Calculated frontier orbital's energy differences have shown a trend identical to experimentally determined values by electron spectroscopy. The participation of EWG in π -conjugation decreases the LUMO level, the energy gap of derivatives and changes distribution of LUMO from whole π -system (Fig. 2 left) to primarily onto bithiophene part and EWG (Fig. 2 right).

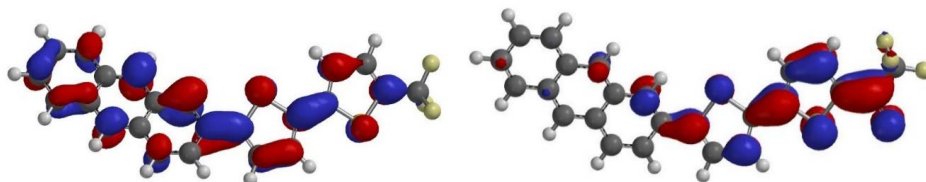


Figure 2 Graphical distribution of LUMO obtained by DTF calculations of **IIIA** (left) and **IIIB** (right).

Table 1 Comparison of theoretical and experimental values of frontier orbital levels of derivatives **IIIA,B**.

	ΔE_g [eV] theor.	ΔE_g [eV] exp.*	E_{LUMO} [eV] theor.	E_{LUMO} [eV] exp.**
IIIA	3.11	2.76	-2.17	-2.65
IIIB	2.71	2.46	-2.73	-2.72

* from UV/VIS spectroscopy; ** from cyclic voltammetry

Transient electronics for edible neuroprosthetics

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Transient electronics is a recent challenging research field aiming at the realization of functional electronic devices able to disappear in a controlled and predefined manner¹. Amongst different applications, biomedical devices based on transient technology have raised a lot of interest^{2,3}. Their ability to dissolve within the biological environment, thus avoiding infections due to a prolonged stay and risks related to surgical retrieval, is their main appealing characteristic. In many cases the device relies on silicon-based electronics, but the incorporation of polymers in the design, mostly as flexible substrate or for drug-release purposes, is becoming more and more exploited⁴. Due to the intrinsic versatility of polymeric materials, which potentially allow for a great variety of customized application and fabrication techniques, fully polymer-based transient electronic devices represent the natural step forward in this research area. We therefore intend to contribute to the progress in the field of transient electronics by fabricating probes for neural signal recording based on biocompatible and biodegradable polymers, both as substrate and active material, thus introducing the edible neuroprosthetics concept. In the specific case, we relied on Polycaprolactone (PCL)⁵ or Poly Lactic-co-Glycolic Acid (PLGA)⁶ as substrate and Poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) as conductive conjugated polymer. With these materials as building blocks, a series of passive neural probes were fabricated and implanted in mice brains (visual cortex area) to assess their *in-vivo* durability. Several time-points (1, 3, 6 and 9 months) have been established for the implants analysis in order to have a better comprehension of the degradation process within the biological environment and the response of the biological environment itself to the insertion of an external object. Preliminary results show that after one month of implantation the astrocytes are visibly activated as expected, whereas there is no evidence of activated microglia. In the near future, implantation of active neural probes will give insight also on the recording capacity of the devices.

This work was supported by European Commission (project № 701632).

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Atomic Layer Deposition of ZnO for Top Cathode Interlayers in Organic Photovoltaics

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Interlayers in organic photovoltaics (OPVs) are used to reduce energy barriers for charge injection/extraction, act as optical spacers, introduce carrier selectivity and increase organic/contact compatibility. To date, the most widely used inorganic interlayers are metal oxides such as TiO₂, ZnO. However, these materials require harsh deposition conditions and hence are generally used in inverted devices. Here we will show, for the first time, that proper selection of materials and conditions allow the use of an Atomic Layer Deposition (ALD) system to deposit thin conformal ZnO interlayers on bulk heterojunctions (BHJs).

ALD is a surface limited technique for layer-by-layer growth of uniform and conformal coatings by nucleation of gas phase precursors on OH-reactive surfaces. In the case of non-reactive polymers, the precursors diffuse into the polymer film. To avoid this diffusion and encourage surface deposition, we selected BHJ with a high T_g polymer and high fullerene content. By controlling the number of ALD cycles and temperature we were able to grow a thin, conformal ZnO film on PCDTBT:PC70BM, as shown in Fig. 1.

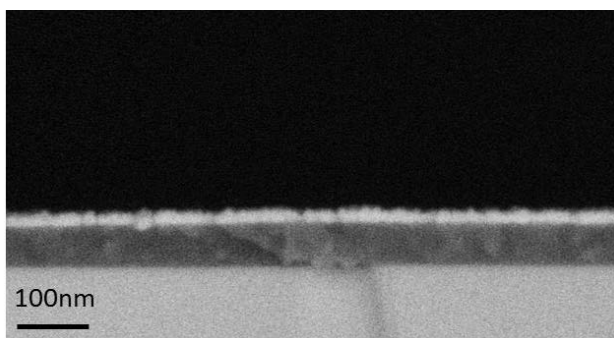


Fig. 1. Cross section BSE HRSEM micrographs of PCDTBT:PC70BM (1:4 %Wt) BHJ on Si substrate after exposure to 130 ALD cycles at 60°C.

The ALD-ZnO interlayer was utilized in OPVs and compared to similar devices with solution deposited ZnO nanoparticle (np) interlayers. The photocurrent density, J_{sc}, is higher for devices with ALD-ZnO but the open circuit voltage, V_{oc}, is lower. The low V_{oc} is associated with the poor ZnO crystallinity which induces a barrier for charge extraction. To recover the V_{oc} we introduced a fluorinated phosphonic acid additive to the blend. The additive segregates to the film surface, interacts with the ZnO and shifts its work function effectively increasing V_{oc}. Additive addition also increases J_{sc} by passivating the dangling bonds and surface states of ZnO. Overall, the best device produced with the additive and ALD-ZnO poses power conversion efficiency of 3.5%, which is significantly higher than that of the best np-ZnO device, 2.7%.

Synthesis of furan/phenylene co-oligomers for organic electronics.

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The optical and electronic properties of thiophene-based π -conjugation molecules have been exclusively studied as perspective materials for optoelectronic applications. Nevertheless furan-contained π -conjugated materials e.g. α -oligofurans has been shown to be perspective alternative materials for organic electronics due to their higher rigidity, higher fluorescence, increased solubility and comparable to thiophene-based materials semiconducting properties¹. Another important aspect is that furan-contained scaffolds potentially can be obtained from renewable sources and are considered to be biodegradable². Moreover furan/phenylene co-oligomers have been shown to have efficient luminescent properties, and application in organic light-emitting and single crystal field-effect transistors^{3,4}. Therefore the development of synthesis of furan-contained π -conjugation co-oligomers is fundamental challenge on the way toward improved organic materials for optoelectronic applications. Herein we developed a universal synthetic strategy approach to alternated furan/phenylene co-oligomers with variable π -conjugation backbone.

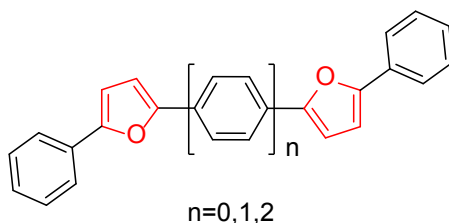


Fig. 1. Obtained furan/phenylene co-oligomers.

Targeted molecules with 1,4-benzene and 4,4'-biphenyl central linker were synthesized by combination of Stille, selective bromination, and followed Suzuki cross-coupling reactions. However, compounds with 2,2'-bifuranyl central π -linker were obtained by another synthetic approach included the oxygen promoted Pd-catalyzed homocoupling of 2-arylfurans. Synthesized furan/phenylene co-oligomers were studied by optical and fluorescence spectroscopy and showed remarkable photoluminescence properties both in solution and solid state. Cyclic voltammetry measurements reveal that furan/phenylene co-oligomers have first reversible oxidation peak that means that they are stable upon multiple Red/Ox cycles which is highly favorable for charge transport. The thermal stability was investigated by TGA and DSC analysis. Furan/phenylene co-oligomers have been shown to be stable at inert atmosphere and do not show any signatures of decomposition up to melting point at oxidizing atmosphere. The photostability in solution and solid state is also discussed.

This work was supported by RFBR (project № 16-33-60011 mol_a_dk).

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Highly Efficient All-Inorganic Planar Heterojunction Perovskite Solar Cells Produced by Thermal Co-Evaporation of CsI and PbI₂

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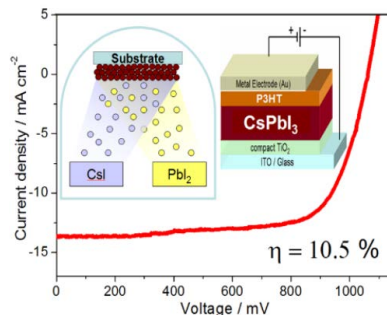
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Hybrid organo-inorganic “perovskite” solar cells have attracted a great interest of the research community due to their simple architecture and easy production technology, low cost of raw materials and record-breaking power conversion efficiencies exceeding 20% for the best laboratory devices.¹ Yet remarkably, perovskite solar cells have not been implemented on industrial scale. While several factors may hinder the development, primary obstacle is the poor stability of perovskite materials with respect to the elevated temperatures, moisture, oxygen², electric field and light exposure,³ resulting in poor device operation lifetimes. This limitation provides impetus for designing improved generations of perovskite absorbers to enable long-term operation stability of the solar cells. Replacing fragile organic moieties with robust inorganic cations can be considered as a promising approach to designing more stable materials. While some inorganic lead-halide perovskites CsPbX₃ (X=I, Br) have shown enhanced resistance towards moisture in combination with improved thermal and photochemical stability,⁴⁻⁵ their photovoltaic performances are still inferior as compared to the classical hybrid perovskites (e.g. MAPbI₃). Here we report all inorganic CsPbI₃ planar junction perovskite solar cells fabricated by thermal co-evaporation of CsI and PbI₂ precursors. The best devices delivered power conversion efficiency (PCE) of 9.3%-10.5% thus coming close to the reference MAPbI₃-based devices (PCE~12%). These results emphasize that all inorganic lead halide perovskites can successfully compete in terms of photovoltaic performance with the most widely used hybrid materials such as MAPbI₃.



This work was supported by RFBR (project № 16-03-00793) and Skoltech-MIT NGP collaboration program.

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Inkjet printing of organic semiconductor materials and devices

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Printing technologies provide great opportunities for rapid and low-cost technology of electronic devices. This technology especially useful for creation of individual devices because it does not require the shadow masks as for thermal vacuum evaporation and photolithography. Solutions of organic polymeric semiconductor materials are the most interesting for printing because they may be used for creation of different semiconductor devices. There are special requirements (viscosity, surface tension, particle size, pH) for inks used for inkjet printing. At the same time, inkjet printing process requires careful adoption of operating modes of the printer heads for different inks. Computer experiment allows facilitate this work, and helps to understand how different parameters affect the process of droplet formation. Therefore, the aim of this work is to simulate the process of inkjet printing of organic materials based on semiconducting polymers.

Simulation was carried out in the specially designed program based on the model developed in ^{1,2}. Printing was performed on the inkjet DOD printer Dimatix DMP-2831 (Fujifilm), rheological characteristics were determined with rheometer DVT3T-LV+CP (Brookfield) and surface tension – with DSA 25E (Kruss).

Simulation of acoustic response of the inks driven by pulse in pump chamber of print head was carried out. It was shown the dependence of maximum printing frequency as function of viscosity, density and sound velocity in the medium. Organic inks based on semiconductor polymeric solutions satisfied for print-head requirements were created. Organic light-emitting devices were printed.

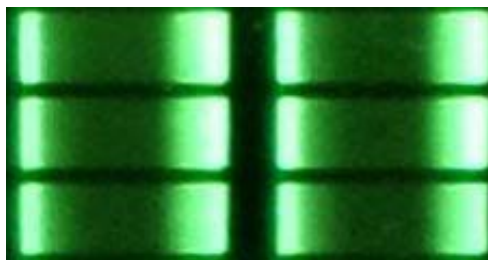


Fig.1. Printed light emitting device

The work is performed in the framework of the grant № 15-12-00034 of Russian Science Foundation.

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Control of Structure and Morphology of Printed Thin Film Organic Field-Effect Transistors

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Organic-based devices have long been desired for next-generation electronics due to its features, such as flexibility, large area coverage or low cost processing. Organic field-effect transistors (OFET) have many potential applications like a variety of sensors for biological, vapour or pressure, or small electronic circuits for which are very close to commercial viability. However, a higher control of morphology and structure for solution processed organic thin films is crucial for OFETs reproducibility. Therefore, engineering processing techniques that could lead to highly crystalline and homogenous semiconducting thin films for high reproducibly OFETs is a current challenge. In this work, bar-assisted meniscus shearing (BAMS) technique of organic semiconductor blends based on small semiconducting molecules and the binder polymer polystyrene (PS) is presented^{1,2,3}. This technique gives rise to highly crystalline and isotropic thin films, which are suitable for OFETs with high mobility, high on/off ratio and near-zero threshold voltage. Moreover, we report the influence of the deposition parameters and solution formulation on the thin film polymorphism and morphology, and its impact on the device performance.

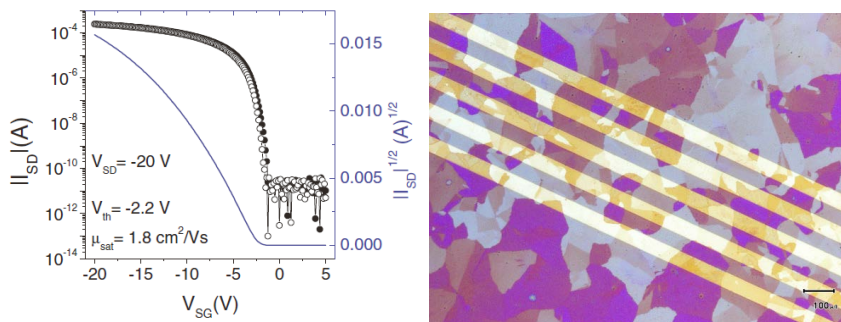


Fig. 1. (left) Transfer characteristic of OFET fabricated by BAMS. (right) Optical microscope image of high crystalline thin film deposited by BAMS.

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Effect of alkyl chain length of double-caged fullerene acceptors on photovoltaic performance

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Efficient synthetic route to tightly bound double-caged [60]fullerene derivatives has been developed through lithium salt-assisted [2+3]-cycloaddition. The bispheric molecules feature rigid linking of the fullerene spheres via a four-membered cycle and a pyrrolizidine bridge with an ester function CO₂R, which can be varied due to easy accessible starting glycine ester.

Here we report a series of such double-caged fullerene derivatives with alkyl substituent (hereinafter, d[60]FR, Fig. 1), which have been prepared and characterized by UV/Vis- and NMR spectroscopy, X-ray diffraction, cyclic voltammetry.

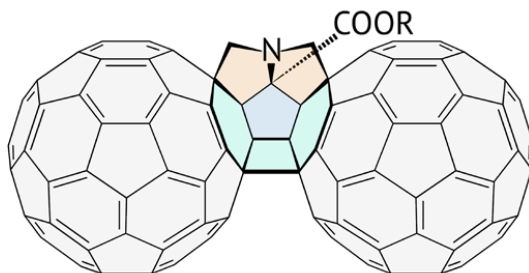


Fig. 1. Structure of double-caged fullerene derivatives

Variation of the ester alkyl chain significantly improves solubility without affecting the electronic properties. Cyclic voltammetry studies revealed three closely overlapping pairs of reversible peaks due to consecutive one-electron reductions. Rigid pyrrolizidine and cyclobutane moieties provide tight linkage of the two fullerene cages thus enhancing intramolecular electronic communication and ensuring small reorganization energy. X-Ray diffraction analysis shows that the coordination number of d[60]FR equals 9, which is higher than in the PCBM single crystal without solvent impurities (7)¹.

An application of double-caged fullerenes in OSC allowed a two-fold increase in power conversion efficiencies of as-cast P3HT/d[60]FR devices compared to the P3HT/PCBM ones. This is attributed to their good solubility and enhanced charge transport properties, both intramolecular, due to tightly linked fullerene cages, and intermolecular, due to large number of close contacts between the neighboring double-caged molecules. Surprisingly low optimal content of double-caged fullerene acceptor in the photoactive layer (ca 30 wt%) favored better light harvesting and carrier transport due to larger content of P3HT and its higher degree of crystallinity. The reported results suggest good potential of the novel doubled-cage fullerene derivatives with customizable alkyl chain as acceptor materials for organic electronic devices.

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Ambipolar 1,8-naphthalimide derivatives exhibiting aggregation enhanced emission phenomenon

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Organic materials with a tetraphenylethene (TPE) moiety are widely applied in an array of fields ranging from biosensing to optoelectronic systems as they are characterized by strong photoluminescence in solid state comparing to that observed for solutions¹. Emitters with aggregation enhanced emission (AEE) phenomenon are used for the fabrications of organic light emitting diodes (OLEDs) since their emission is enhanced in the solid state¹. In addition to high photoluminescence quantum yield (PLQY) in the solid state, emitters for OLEDs should have possibility to transport charges so effectively that holes and electrons recombine emitting light after reaching the emitting layer². Donor and acceptor moieties can be combined in one molecule to get both high efficient photoluminescence and ambipolar transport of organic emitters in solid-state for OLEDs.

With the aim to develop efficient emitters for OLEDs, we have studied the photo- and electro-physical properties of three new TPE substituted 1,8-naphthalimide derivatives with the TPE as a donor and 1,8-naphthalimide as an acceptor. These compounds were found to be capable of transporting both holes and electrons. The hole and electron mobilities for the studied compounds were found to be in the range from ca. 4.1×10^{-5} to 2.3×10^{-3} cm²/Vs at electric fields from 1.6×10^5 to 6.4×10^5 V/cm. The shapes of the time-of-flight (ToF) current transients revealed the low dispersive electron and dispersive hole transports in the layers of the compounds. Ionization potentials of the solid samples of the compounds were estimated by electron photoemission spectroscopy, which gave values in the range from 5.76 eV to 5.9 eV.

For the estimation of AEE activity of the new compounds the fluorescent behavior of their dilute dispersions in the mixture of THF and water with the different water fractions were studied. The emission of the THF solutions of the studied derivatives was weak, however, an enhancement in luminescence intensity was observed with the increase of the concentration of water. Since the studied derivatives are insoluble in water, the increase of the water fraction in the mixture of solvents leads to the reduction of the number of the dissolved molecules of the compounds. The emission of the 50:50 (v/v) water/THF mixture of the derivatives was extremely low. The enhancement of luminescence intensity was observed with the further increase of water fractions. In addition, the intensity maxima of PL spectra (λ_{\max}) were shifted to the red region. For example, for one of the studied compounds λ_{\max} was observed at 522 nm for the 10:90 water/THF mixture while λ_{\max} at 630 nm was recorded for the 90:10 water/THF mixture.

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Probing of luminescent dopants in single-crystal thiophene-phenylene and furan-phenylene co-oligomers by photothermal deflection spectroscopy

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Single-crystal thiophene-phenylene (TPCO) and furan-phenylene co-oligomers (FPCO) have a great potential for the application in optoelectronics and photonic devices, since they can combine high luminescence and efficient charge transport. The promising approach to control the luminescent properties of organic semiconductor crystals is their doping by highly luminescent molecules¹. Recently, we have found that these luminescent dopant molecules can appear as byproducts in the course of TPCO chemical synthesis^{2,3}.

In this work, we report on study of luminescent dopants in single-crystal TPCO and FPCO. Photothermal deflection spectroscopy⁴ which can probe very low amount of impurities via their absorption in the transparency range of the material (Figure 1a). The TPCO and FPCO crystals were grown from the vapor phase and from solution.

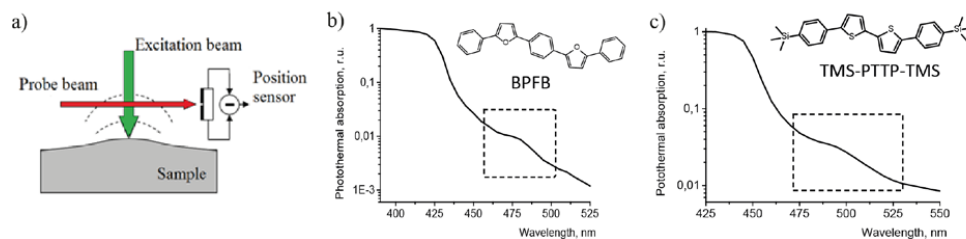


Fig. 1. a) Experimental scheme of photothermal deflection spectroscopy; b) Spectrum of BPFB crystal (from solution); c) Spectrum of TMS-PTTP-TMS single crystals (from vapor phase). The impurity absorption bands are selected by rectangles.

We detected the dopant absorption features in the TPCO and FPCO single crystals samples (Fig. 1b, Fig. 1c). Taking into account the TPCO and FPCO photoluminescence data, we discuss the sensitivities of luminescent and photothermal techniques to small amounts of dopants.

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Fluorescent properties of salt built of 3-cyano-4-dicyanomethylene-5-oxo-4,5-dihydro-1H-pyrrole-2-olate anion and 2-aminopyridinium cation

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The production of cocrystals of organic molecules is a direction in crystal engineering which has recently attracted a lot of interest in connection with the development of new functional materials with unusual optoelectronic properties. On the one hand, design of cocrystals opens the prospect of a purposeful change in the packing of molecule responsible for certain property in order to tune this property. This is possible thanks to a large number of organic molecules which can form cocrystals with the key molecule. On the other hand, design of cocrystals opens the possibility to combine several properties from different molecules in one crystal simultaneously. However in cocrystals of organic luminophores there is a problem of the total energy transfer from a component that emits in short-wavelength region to a component that emits in long-wavelength region. This caused several unsuccessful attempts to make crystals of salts comprised by cation and anion, which possess complementary emission^{1,2}. Nevertheless there is one example of salt in which both centres luminesce – this is a mixed salt of new organic anion 3-cyano-4-dicyanomethylene-5-oxo-4,5-dihydro-1H-pyrrole-2-olate (HA^-), its deprotonated form (A^{2-}) and cadmium cation Cd^{2+} : $[\text{Cd}_3(\text{HA})_2(\text{A})_2(\text{H}_2\text{O})_{10}] \cdot 0.5\text{H}_2\text{O}$ ³. In crystals of this salt dianion A^{2-} emits in short-wavelength region (377 nm), anion HA^- emits in long-wavelength region (620 nm). Therefore it is possible to design crystals of organic salt, in which one ion emits in short-wavelength region and the other emits in long-wavelength region (ideally in two complementary spectral regions). One needs only to define a specific packing of ions in crystal necessary for this. Salt built of anion HA^- and cation 2-aminopyridinium (APY^+) has been chosen to solve this problem. Fluorescence spectrum maximum of HA^- in crystal lies in range of 544-669 nm depending on its molecular surroundings⁴. Fluorescence spectrum maximum of APY^+ lies near 367 nm⁵. The salt was synthesized, three types of crystals with composition APY^+HA^- , $\text{APY}^+\text{HA}^- \cdot \text{H}_2\text{O}(\alpha, \beta)$ were obtained and their crystal structures were determined using single crystal x-ray diffraction, their fluorescent spectra were recorded. It turned out that in all types of crystals fluorescence of cation APY^+ was absent. Water solution of this salt as well as filter paper saturated with this salt gave clear peak of cation fluorescence. For three types of crystals wavelength of fluorescence spectrum maximum of HA^- is correlated with crystal structure. Attempt to disclose an effect of substrate on cation fluorescence in APY^+HA^- salt is made.

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Nickel oxide as hole contact material in organic electronics: the role of surface chemistry and microstructure

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Transition metal oxides, like nickel oxide (NiO), have been widely used as carrier selective buffer layers in hybrid solar cells. However, the surface and stoichiometry of NiO films depend strongly on various deposition parameters and have strong impact on the electronic properties of the prepared NiO layers. Nanometer thin nickel oxide layer (sNiO) were grown by casting a precursor solution of nickel acetate tetrahydrate 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 compact nickel oxide films exhibit high reactivity and low p-type conductivity after oxidation in ambient air. While post-annealing in an oxygen deficient environment reduces excess interstitial oxygen, shifting the Fermi-level of the sNiO film further into the bandgap, the increase in oxygen partial pressure under ambient atmosphere does not lead to a higher p-doping level. Temperature, plasma treatment and molecular modification dramatically change the surface properties. We address the crucial roles of nickel hydroxide (Ni(OH)₂) and nickel oxyhydroxide (NiOOH) groups for the electronic properties of the NiO layer. Finally, our analytical results are correlated to the device performance of organic flat- and bulk-heterojunction solar cells.

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Time-Dependent Recombination Orders in Organic Disordered Semiconductors

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Charge carrier recombination in organic disordered semiconductors is strongly influenced by thermalization of charge carriers in the density of states (DOS). Measurements of recombination dynamics, conducted under transient or steady-state conditions, can easily be misinterpreted when a detailed understanding of the interplay of thermalization and recombination is missing. To enable adequate measurement analysis, we solve the multiple-trapping problem for recombining charge carriers and analyze it in the transient and steady excitation paradigm for different DOS distributions.

We show that recombination rates measured after pulsed excitation are inherently time-dependent, since recombination gradually slows down as carriers relax in the DOS. When measuring the recombination order after pulsed excitation, this leads to an apparent high-order recombination at short times. As times goes on, the recombination order approaches an asymptotic value. For the Gaussian and the exponential DOS distributions, this asymptotic value equals the recombination order of the equilibrated system under steady excitation. For a more general DOS distribution, the recombination order can also depend on the carrier density, under both transient and steady-state conditions.

We conclude that transient experiments can provide relevant information about equilibrium recombination and the underlying DOS occupation provided that consistent modelling of the system is performed.

This work was supported by the German Federal Ministry of Education and Research (Project UNVEiL) and the German Research Foundation (Project LE 747/48-1).

Organic electrochemical transistors (OECT) prepared via screen printing technique as a tool for biosensing

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Among all the devices that has risen in the field of bioelectronics, organic electrochemical transistors (OECTs) show promising characteristics for bio sensing. The key idea is to prepare a matrix of 96 working devices by screen printing method that would be capable to sense electrical response of cardiomyocytes. It was published that cardiac cells are highly sensitive toward new drugs. Such a device would be ideal for monitoring of toxicity of these drugs.

Advantage of screen printing is the capability of preparation of highly patterned individual layers. The first layer is formed by silver conductive busbars that with conductive nodes for characterization of performance of the transistor and source/drain (S/D) electrodes. The second layer is made up of semiconducting polymer (poly(3,4-ethylenedioxythiophene) doped with poly(styrene sulfonic acid) (PEDOT:PSS) which creates the channel and gate electrode (G). Whole device is encapsulated by elastomer to protect cardiomyocytes from contact with silver layer. The architecture of our OECTs is planar. All these steps were conducted by screen printing machine RokuPrint SD 05.

Printed electrochemical transistors were characterized by measurement of output and transfer characteristics in phosphate buffer saline (PBS). An example of such a measurement can be seen in Fig. 1, which shows typical transistor characteristic.

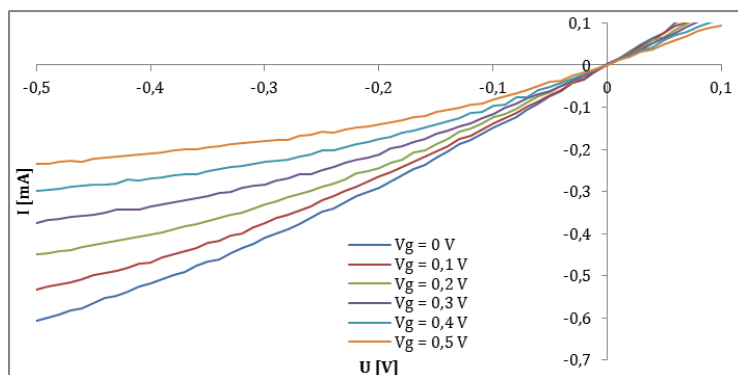


Fig. 1 Output characteristics of printed OECT

The homogeneity and thickness of layers and S/D geometry are crucial parameters that affect the behaviour of devices. It is clear that for improvement of our printed devices the dimensions of the channel need to be miniaturized to enhance a signal.

This work was supported by Czech Science Foundation via project No. 17-24707S, research infrastructure was supported by projects MŠMT No. LO1211 and FCH-S-16-3393.

Effect of the substrate and processing conditions on the photochemical, thermal and electrochemical stability of the MAPbI₃ thin films

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Exploration and implementation of the renewable energy sources attract steadily increasing attention of the research community and industry worldwide. Perovskite solar cells represent a highly promising emerging photovoltaic technology. Recently, power conversion efficiencies of the best laboratory samples of lead halide based perovskite solar cell have exceeded 22%. While the efficiencies are that impressive, the stability of the perovskite solar cells under the realistic operation conditions is rather disappointing. Improving stability of perovskite photovoltaics represents a big challenge and success in mechanistic understanding and prevention of the major degradation processes is crucial for commercialization of this technology.

In the present work, we report a systematic analysis of the intrinsic photochemical, thermal and electrochemical stability of MAPbI₃ films grown on different substrates under a variety of processing conditions. The degradation behavior of the perovskite films was monitored under anoxic environment inside the glove box (O₂, H₂O < 0.1 ppm). We have applied a set of complementary techniques involving absorption UV-Vis-NIR spectroscopy, scanning electron microscopy (SEM), X-ray diffraction analysis (XRD) and EDX microanalysis to reveal evolution of the chemical composition and structure of the material under the aforementioned stress conditions.

The obtained comprehensive set of the experimental data allowed us to propose some pathways of the thermal, photochemical and electrochemical degradation of the perovskite films.

This work was performed in the frame of the Skoltech-MIT NGP program.

Iodine-doped carbon nanotube–polyimide composites for microelectronics

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The use of carbon nanotubes (CNT) to increase the conductivity of polymers, as an alternative of carbon black, was shown¹. Current research aimed to obtain composites for specific applications, for example, photovoltaic devices or supercapacitors. In many cases, even improving mechanical properties, due to using nanotubes as fillers, is useful. Despite the fact that the CNT-polymer composites have very low percolation thresholds, their electrical conductivity is still not very high. The doping of the carbon nanotubes leads to a strong increase in conductance due to changes in the electronic structure caused by charge transfer². In our research institute were made polyimide-based composites with different contents of single-walled CNT. CNTs were uniformly distributed in the polyimide matrix. Composite materials showed high values of thermal resistance and resistance to thermo-oxidative degradation, and good mechanical properties³.

Stable air iodine doped CNT-polymer composites show an increase in conductivity 2-5 times compared to composite materials with undoped CNTs on the same polymer matrix, was shown⁴. Analysis of the temperature-conductivity dependence indicates the tunneling mechanism of conductivity in iodine doped polymer-CNT composites caused by the temperature change.

The aim of our work is to develop a simple environmentally friendly technology of conductive composite materials based on polyimide filled CNTs doped with iodine. The developed technology may find application in the microelectronics production, such as OLEDs, solar cells, flexible printed circuit boards thin film field effect transistors, photovoltaic devices, etc.

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Small- and large-signal analysis of relaxation times in pentacene diode

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Organic electronics devices based on small molecule or polymer materials, like organic field effect transistor (OFET), organic light emitting diode (OLED) and organic solar cells (OSCs) have attracted a great attention due to their application as light weight and flexibility. The understanding of the electrical conduction mechanism in these materials and at their interfaces represents a challenge¹. In the organic electronic devices, metal-organic semiconductor interface and charge transport through organic semiconductor play a major role in determining the electrical transport².

There are several experimental methods exists for characterization of defect states in semiconductors, but most of them allow only an indirect conclusion on the energy distribution. One of the most used methods is a deep level transient spectroscopy (DLTS). DLTS is assumed as a technique for observation and characterization of deep levels present in the bandgap of semiconductors³ although it is actually only transient capacitance (TC) measurement. This method is based on the study of time-domain response after application of larger excitation signal and it is sensitive also to defects as well as interface charging. Another very common method is the impedance spectroscopy (IS) which is running a small AC probe signal at the specific DC voltage bias to probe a local behaviour. Even though usually these experimental techniques give different results, both of them are correct since the measurement conditions differ.

In this study, we have investigated the impact of the excitation pulse on the evaluation of the charge relaxation in organic diode, where the organic semiconductor (pentacene) film is sandwiched between two conductive electrodes (copper and aluminium Fig. 1.(a)). The small- and large-signal analysis (Fig. 1.(b) and (c)) are compared and the transition between them is shown to illustrate the relaxation time reliability.

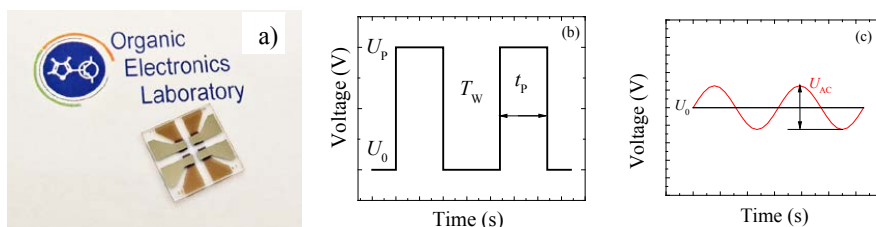


Figure 1: (a) Photo of fabricated device. The temporal evolution of applied voltage for (b) TC and (c) IS.

This work was supported by the Slovak Research and Development Agency (grants APVV-14-0739 and APVV-14-0740).

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Synthesis, characterization and photovoltaic properties of new iridium-containing conjugated polymers.

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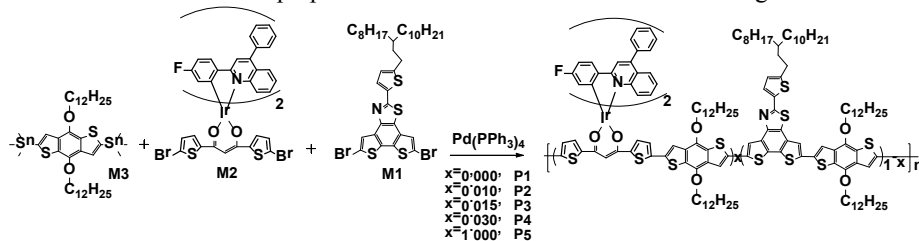
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Novel donor-acceptor (D-A) copolymers **P1** - **P5** with iridium-complexed moieties in their side chains have been prepared on the base of new iridium-containing monomer **M2**.



Scheme 1.

M_n and M_n/M_w of the polymers **P1-P5** are in the range of 48700-72600 kDa and 2.25-3.20, respectively. Optical bandgaps of **P1-P5** are in the range of 1.96-2.08 eV, respectively. HOMO and LUMO energy levels of the polymers **P1-P5** were estimated from CV and are of -5.21, -5.21, -5.18, -5.17, -5.42 eV and -2.93, -3.00, -2.99, -2.92 - 3.08 eV, respectively. BHJ polymer solar cells were developed based on blend compositions (**P1-P5**):PC71BM. The values of J_{sc} , V_{oc} , and FF are in the ranges of 0.95-4.44 mA/cm², 0.67-0.69 V and 34.6-56.8%, power conversion efficiencies (PCE) are in the range of 0.22-1.74%, respectively. Increasing of the photovoltaic parameters was achieved with increasing of iridium complexes percentage in the polymers due to involvement of triplet effects. The improvement in the efficiency of the triplet-forming polymers **P2** and **P3** in comparison with **P1** appears to be due to the formation of triplet excitons in comparison with singlet excitons in the polymer **P1** which does not contain heavy metals. Triplet-forming polymers interfere with the recombination of the geminal pairs and have a longer exciton lifetime and, as a consequence, a longer exciton diffusion length, thereby increasing the percentage of excitons reaching the donor / acceptor interface, that is, the efficiency of generation of charges and photocurrent. Indeed, the triple-forming polymers **P2** and **P3** containing iridium complex exhibit larger values of the short-circuit current at an almost identical values of the open circuit voltage and the filling factor in comparison with **P1**. With further increase in the content of iridium complex fragments in polymers, for example up to 3 mol% for polymer **P4**, the efficiency falls to 1.23%. PCE, J_{sc} , FF based on **P5** with 100% mole of the Ir complex content decreased to a minimum value of 0.22%, 0.95 mA/cm² and 34.6%, respectively. This may be due to a decrease in the charge transfer properties of polymers with an increase in the content of the iridium complex, which breaks the conjugation of the polymer chain and further reduces the mobility of charges careers, which leads to a decrease in the short-circuit current in the device. The obtained results show the prospects of this approach for the design of narrow-band conjugated triplet-forming polymers containing iridium complexes in the side chain with the aim of increasing the efficiency of solar energy conversion.

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Description of charge-carrier transport in crystalline organic semiconductors beyond simple hopping or band-transport models

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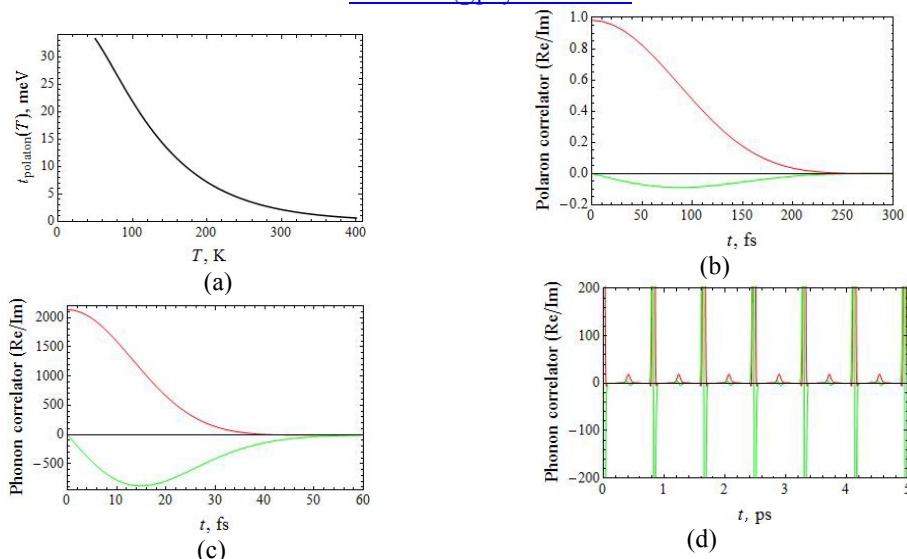


Fig. 1. (a) The band narrowing effect, in terms of polaron transfer integrals dressed by phonons; (b, c, d) typical polaron and phonon correlator profiles on different time scales. All plots are for simple cubic lattice, $T = 300$ K, NN hopping integrals $t = 100$ meV, and 3 vibronic modes per site

Adequate description and efficient computation of charge-transfer properties of realistic organic materials constitute one of the major challenges of ongoing materials research for organic electronics. A powerful strategy for this challenge is presented by multiscale modeling¹, which combines a series of models and computational methods working on different spatial scales, from the atomic to the mesoscale and the scale of an actual device.

Within the multiscale modeling methodology, we calculate charge-carrier mobilities of small-molecule organic crystals, accounting for polaronic effects. Starting from transfer integrals and electron-vibron couplings extracted from DFT simulations of single molecules and small crystalline samples, we then study the Holstein–Peierls model of a crystal thus parametrized. Following a recently developed approach² within the latter model, we extend the mean-field polaron theory to beyond the small-polaron approximation, so that polarons form bands (see Fig. 1(a)). This lets us probe the parameter region between the hopping and band-transport regimes, where the mobility may drastically increase, due to a non-trivial interplay between the so-called polaron and phonon correlators^{1,2} (see Fig. 1(b, c, d)).

The method and its implementation we have developed are to be further applied to materials used in organic field-effect transistors and solar cells, as well as biocompatible materials.

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Synthesis of hyperbranched oligophenylenes with phenylene ethynylene fragments for optoelectronics

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The synthesis of oligophenylenes with phenylene ethynylene fragments was carried out following the Sonogashira reaction. The polyphenylenes containing one and two benzene rings as the internode fragments were studied to elucidate the influence of conjugated fragments of different lengths, as linkers for the branching centres on optical properties. The oligophenylenethynylenes structure is confirmed by combining NMR-spectroscopy and photophysical characterization and also compared to the spectra of model building blocks compounds.

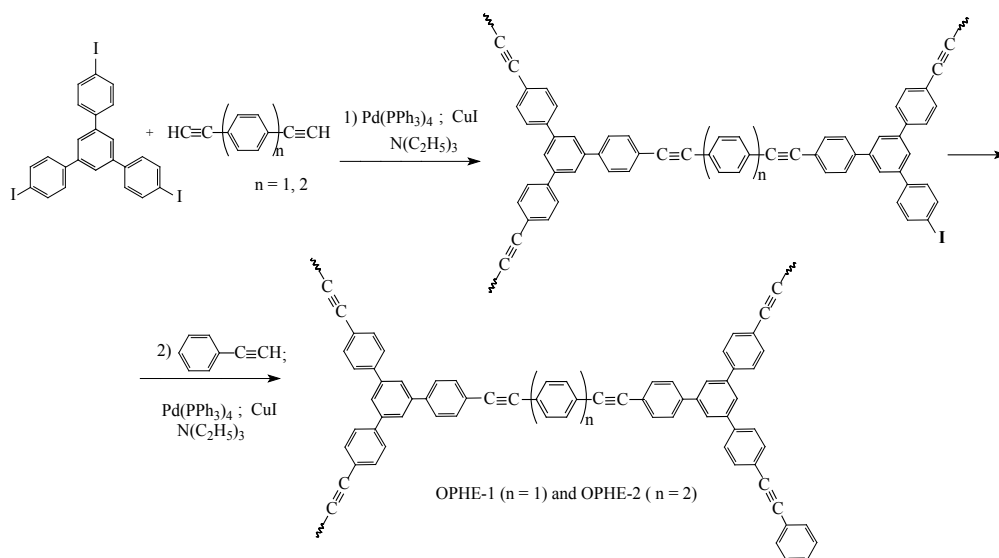


Figure 1. Scheme of Sonogashira reaction showing the synthesis of branched oligophenylenethynylenes with phenylene or biphenylene moieties

Branched oligomers are good ultraviolet emitters in solution, while in solid-state aggregation phenomena affect emission performance. A possible application of the representative branched oligomer as high hole mobility interlayer ($\mu_h = 3 \times 10^{-3} \text{ cm}^2/\text{Vs}$) in well-established phosphorescent organic light-emitting (PHOLEDs) device is proposed. Corresponding PHOLEDs performance are compared to devices embedding more conventional hole transporting layers (like polyvinylcarbazole).

This work was supported by project Giovanella/Khotina – the scientific cooperation agreement between CNR and Russian Academy of Sciences (project № 15-53-78042 and RFBR project № 16-03-00425).

New highly potent vacuum- and solution-processable [3]-radialene-based molecular p-dopant: synthesis and application

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Molecular p doping of organic semiconductors is a charge transfer process which occurs upon admixing of organic semiconductors with organic molecules having high enough electron affinity. Molecular doping is widely used in both academia and industry for enhancing the efficiency of various organic electronic devices. For example, the introduction of heavily doped organic layers nearby the electrodes facilitates charge injection thus greatly improving the operation of solar cells and organic light emitting diodes (OLEDs) up to a level acceptable by industry and therefore this concept is used for fabrication of AMOLED displays in smartphones. Most of molecular dopants used for the p-doping of small-molecule and polymer semiconductors are fluorinated derivatives of TCNQ or TCNNQ and they have insufficiently deep LUMO levels (in -5.1 - 5.4 eV range) to dope many useful organic semiconductors. In this contribution, we will report synthesis and characterization of a [3]-radialene-based dopant CN6-CP which is the strongest molecular p-dopant reported in open literature so far. CN6-CP exhibits reduction potential +0.78 vs Fc/Fc⁺ (LUMO -5.87 eV, which is 0.6 eV lower than that of the benchmark F4TCNQ).¹ The unprecedentedly high doping strength of CN6-CP allows efficient doping of donor-acceptor copolymers, e.g., diketopyrrolopyrrole-based PDPP(6-DO)2TT (HOMO -5.49 eV). Absorption spectroscopy and EPR confirmed efficient electron transfer from PDPP(6-DO)2TT to CN6-CP. PDPP(6-DO)2TT:CN6-CP films exhibit electrical conductivities up to 70 S/cm which is one of the highest reported conductivity for molecularly doped polymers soluble in organic solvents. CN6-CP shows a relatively good thermal stability to withstands sublimation in vacuum which makes it potentially suitable for the doping of small semiconducting molecules processed by vacuum evaporation techniques. The superior electron affinity of CN6-CP significantly broadens the range of semiconductors that can be used in devices in the p-doped state.

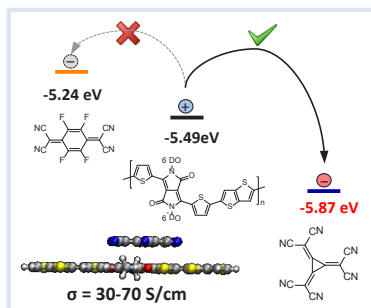


Fig. 1. Structure of F4TCNQ (left), polymer (middle), CN6-CP (right) and schematics of the p-doping process

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Synthesis, theoretical and experimental investigations of new luminescent bithiophenesilane dendrimers

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A search for new materials and the ability to control the spectral-luminescence characteristics according to the particular application requirements is one of the challenging tasks for organic optoelectronics and photonics today. Therefore, of particular interest are new highly efficient organic luminophores, branched and dendritic structures based on them, which possess unique optical properties. In this work, we report on the synthesis and investigation of a number of new luminescent bithiophenesilane dendrimers of different architectures. The chemical structure of these highly branched molecules can be attributed to one of the types of the so called “Nanostructured Organosilicon Luminophores” (NOLs)^{1,2}. They consist of a number of organic luminophores of two types (donor and acceptor) covalently linked to each other through silicon atoms, which break the conjugation and allow highly efficient intramolecular energy transfer between the donor and acceptor luminophores by Forster mechanism. As a result, NOLs show huge absorption cross-section, large pseudo Stokes shift and high luminescence quantum yields.

The dendrimers synthesized are composed of several bithiophene (2T) donor fragments and a central acceptor group – either oligothiophenophenylene (PTPTP) or diphenylanthracene (DPAnT). The ratio of the donor to acceptor luminophores in the dendrimer is determined by a particular molecular architecture. The estimated efficiency of the energy transfer from the donor to the acceptor luminophores in such dendrimers is 94-98%, while the luminescence quantum yield lies in the range of 80-90% when excited at the absorption maximum of the donor fragments. The theoretical and experimental investigations of spectral-luminescent properties of the dendritic molecules and comparison to their less branched analogs will be reported. A fundamental relationship between the molecular structure and properties of the organosilicon dendrimers will be considered.

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Synthesis and investigation of diaryldiazenes incorporating pyrimidine moiety

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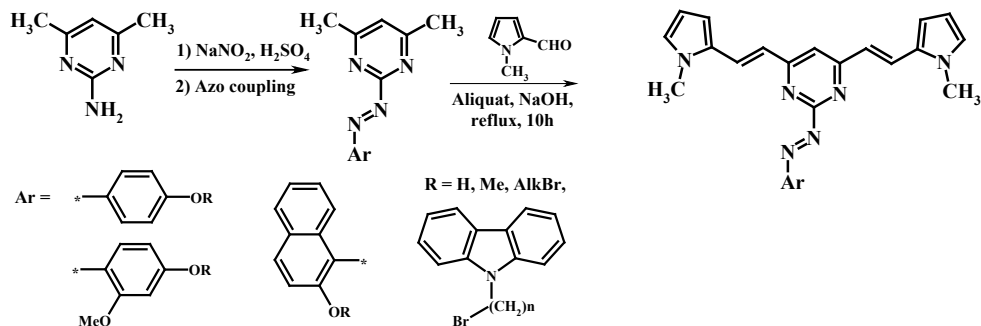
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Functionalization of a pyrimidine ring often affords π -conjugated systems with various interesting properties. Among these compounds push-pull chromophores hold a prominent place as systems with potential photovoltaic properties necessary for application in photo-electronic devices¹. The substituents embedded into the pyrimidine core can tune the character of emission, NLO and two-photon absorption properties. The incorporation of azo linking group into the common conjugation system of a molecule enhance the intramolecular charge transfer thus creating a large delocalized π surface. At the same time, the different spatial arrangement in the azo compounds isomers also affects physical and chemical properties. The E/Z-light induced isomerization of diaryldiazenes in its turn induces a change of the dipole moment. The push-pull structures of this sort can be used in many practical applications such as coloring fibers, materials for electronic devices, NLO materials, reagents in analytical chemistry, *etc.* Additionally, embedding of terminal N-methylpyrrol moieties into the structure of these compounds afford an opportunity of electrochemical polymerization with formation of thin films on the electrode surface. The 4,6-dimethyl-2-aminopyrimidine **1** is an excellent precursor for the preparation of such conjugated systems². Using the synthetic protocol, displayed in the Scheme, we have synthesized a set of some novel 2-azopyrimidines with different edge donor groups. All the prepared compounds were studied in the context of their optical and electrochemical properties.



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Molecular mechanism of reductive dehalogenation by P450 enzymes: possible importance of dissociative electron attachment for biosensor applications

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The molecular mechanism of enzymatic processes induced by cytochrome P450 is of importance for biosensor applications¹ as well as for construction of biological interfaces via immobilization of enzymes in the condensed environment². These interfaces are known to be able to model the drug metabolism under electrochemical conditions³. The electron exchange plays a key role in the P450 catalytic cycle⁴ responsible for reductive dehalogenation of environmental pollutants, including herbicides both in vivo and in electrochemical experiments⁵. It is worth mentioning that enzymatic active centers are hydrophobic in nature, thus containing a very few water molecules⁶. Additionally, the substrate molecule is bound in the active site by weak non-covalent bonds, thus keeping its native electronic structure. Therefore, resonance dissociative electron attachment (DEA) to isolated molecules in vacuo can serve as a model of enzymatic processes under reductive conditions as shown in case of some widely used non-steroidal anti-inflammatory drugs⁷.

The present work reports formation of transient negative ions and their decay for the halogenated herbicides atrazine and bromoxynil studied by means of electron transmission spectroscopy (ETS) and DEA spectroscopy. Dehalogenation of atrazine and bromoxynil is found to be the dominant decay of the temporary molecular negative ions formed at very low (thermal) energies of the incoming electrons. It is concluded that formation of negative ions by electron donation in enzymatic active centers followed by their dissociation along the σ^* bond can be considered as a unifying mechanism of the initial step of reductive dehalogenation catalyzed by P450 enzymes. The present findings attract attention on the role of the resonance electron attachment mechanism in electron-driven enzymatic processes.

The work was supported by RFBR grants (17-03-00196 and 15-29-05786) and by the Italian Ministero dell'Istruzione, dell'Università e della Ricerca.

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Controlling Torsional Rigidity by Introduction of Furan Moiety into Co-oligomers towards Highly Emissive Semiconducting Materials

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The materials based on the chalcogen-containing co-oligomers combining high luminescence efficiency and charge mobility are of great interest for various optoelectronics applications. The incorporation of furan moiety was suggested to increase torsional rigidity and consequently improve both electronic and optical properties. However the relevant insights concerning the intramolecular factors affecting the torsional rigidity in furan/phenylenes as well as in thiophene/phenylene analogues have not been thoroughly investigated yet. Here we study the nature of torsional rigidity and its impact on optoelectronic properties for the alternating furan/ (BPFB) and thiophene/phenylene (AC5) co-oligomers.

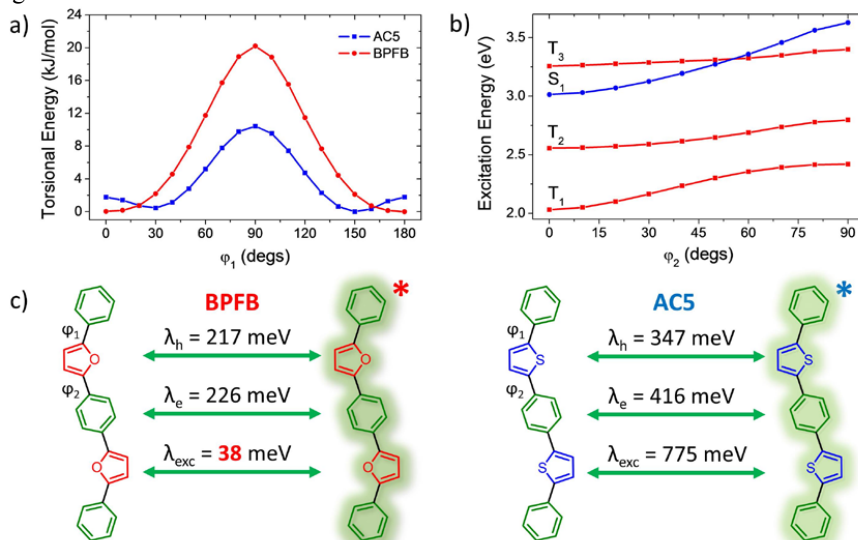


Fig. 1. a) Potential energy surface of S_0 state upon ϕ_1 dihedral angle rotation; b) Conical intersection of S_1 and T_3 states upon ϕ_2 dihedral angle rotation; c) Reorganization energy for hole (λ_h), electron (λ_e) and exciton transfer (λ_{exc}).

We have demonstrated that BPFB is almost twice more rigid than AC5 in both S_0 and S_{1r} states (Fig. 1a), intramolecular interactions having negligible effect on torsional rigidity as compared with conjugation breaking. Higher torsional barrier of BPFB was suggested to impede possible photoluminescence quenching through conical intersection of S_1 and T_3 excited states (Fig. 1b). The higher rigidity of BPFB also lowers reorganization energies for charge and exciton transfer (Fig. 1c).

We conclude that the tuning of molecular rigidity strongly impacts on emission and charge/energy transport being a powerful tool on the way to high performance emissive organic semiconductors.

This work was supported by RFBR (project № 16-33-60011 mol_a_dk).

Filamentary model of resistive switches in composite structures based on organic dyes and colloidal CdSe nanoplates

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Organic resistive memory is being widely studied due to its easy manufacture techniques and suitable operation parameters¹. Composite structures based on organic polymers have attracted attention for resistive memory devices. It was shown in our previous works that resistive switching effect (RS) in polymer based composite materials with organic or inorganic admixtures has high potential for memory applications². Nevertheless, there is still lack of studies with the full description of the physical processes occurring during RS in organic materials. In this work, we present the approach to construction of highly effective memory elements and to control physical processes of RS.

The operation principles of resistive memory presume an ability of system to switch between at least two states “ON” and “OFF” with different resistances. It is widely accepted in the literature that RS mechanism is based on formation and rupture of conducting filament (CF)³. RS speed can be 10 ns, non-volatile, on/off ratio can exceed 2 orders of magnitude, switching electric field is below breakdown values, number of rewriting cycles is 10⁵ or more².

In this work we observed RS in composite structures consisting of polystyrene matrix with incorporation of colloidal CdSe nanoplates, and variation of phthalocyanine-based organic dyes (tert-butyl-substituted bisphthalocyanine of lutetium, tris(hexadecachlorophthalocyanine) of lutetium). Such composition allowed us to obtain not only ON, OFF, but also intermediate stable states. For each state we performed impedance spectroscopy and observed typical single semicircles, which is attributed to the equivalent scheme of parallel resistance R_c and capacitance C . In the intermediate states the value C stays quite stable. After the switch to the ON state the value C increases in more than 3 times. Drastic change in the capacitance is attributed to Maxwell-Wagner (M-W) effect, which could be explained by appearance of structural heterogeneities. This is well explained by CF formation mechanism of RS. In intermediate states only single CF appear and it does not influence on C . In the highest conducting state a system of interwoven CF arises and the M-W effect takes place. Thus by *in situ* impedance spectroscopy we observed the formation of filamentary structure.

The rupture of CF is driven by Joule-heating³ and can be described by 2D elliptic equation in rectangular area, defined by length and radius of CF. Simulations for this model were run, assuming the same geometry device parameters, electric and thermal conductivities and sweep-rate as in the experiments. The results of the simulations fit experimental data, which confirms the reset part of the CF model.

This work was supported by RFBR (project № 16-07-00961, 16-33-60005, 15-03-05890, 16-29-1169).

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A degradation behavior of the polyquinone-based cathode material for lithium-organic batteries

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Design of new energy storage devices possessing high capacity and efficiency represents an important research direction. Organic materials can potentially deliver 200-300% higher specific capacities compared to conventional materials such as LiFePO_4 and even $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$. However, organic materials are often very challenging to handle while forming cathode composites and, most importantly, they show much inferior durability as compared to the mainstream inorganic lithium-ion battery technologies. Therefore, there is an urgent need for a systematic investigation of various organic cathodes, revealing molecular structure-performance-stability relationships and unraveling the main degradation mechanisms.

Here we present the synthesis, experimental and theoretical DFT study of a novel organic polyquinone-based cathode material $(\text{C}_6\text{H}_2\text{O}_2\text{CH}_2)_n$ for lithium batteries. It has been shown that strong electrochemical lithiation of the material upon battery charging becomes irreversible and leads to a rapid deterioration of the device performance. On the contrary, carefully controlled degree of lithium insertion within the defined charge/discharge potential window results in a stable battery operation within more than 150 cycles. DFT calculations have shown that deep lithiation of the material causes a strong conformational reorganization of the polymer domains (Fig. 1). Repeatable expansion and shrinkage of the electroactive material leads to a rapid loss of the cathode integrity and the battery failure.

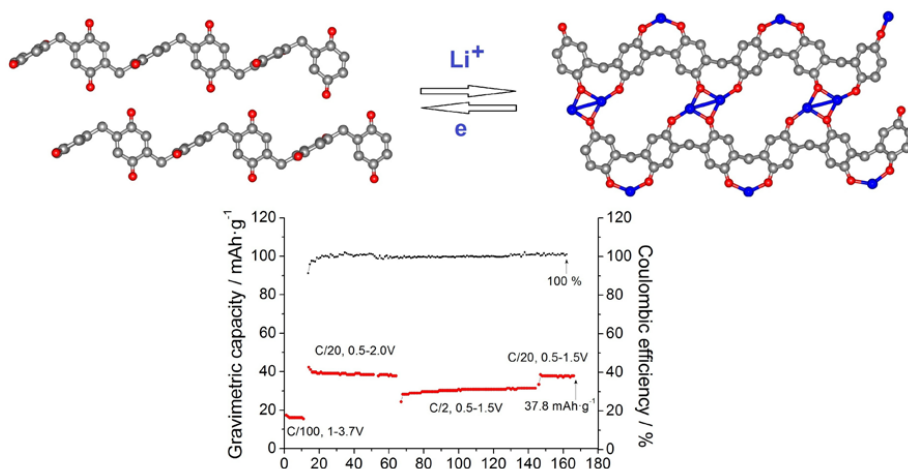


Figure 1. Reversible reorganization of the polymer under lithiation (upper) and the dependence of the discharge capacity and coulombic efficiency of PBQM // Li battery under different cycling rates within the controlled potential windows (lower)

This work was supported by RSF (grant № 16-13-00111).

Linear conjugated oligomers based on 2,1,3-benzothiadiazole as new luminophores for organic photonics.

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Organic electronics is a rapidly developing field of science and technology¹. It relies upon printing technology for creation of different electronic and optoelectronic devices with unique properties, such as flexibility, energy efficiency and low weight². Conjugated oligomers are one of the widely used semiconducting 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 shift³. Such properties of BTZ-based oligomers make it possible to apply them as excellent luminescent materials in various optoelectronic applications.

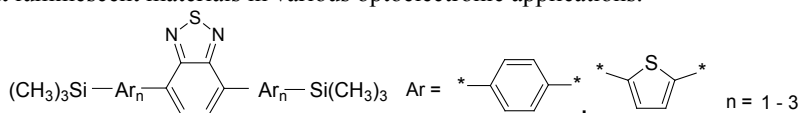


Fig.1. Chemical structure of the conjugated organosiliconoligomers based on BTZ.

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 terminal groups, as well as to study their optical and thermal properties (Fig.1). For the synthesis of novel conjugated organosilicon oligomers based on 2,1,3-benzothiadiazole was used Suzuki-Mayer reaction. This reaction meant interaction with aryl or heteroarylhalide with aryl or heteroarilbororganic compound in the presence of a base and palladium catalyst⁴.

At this stage of research, we have synthesized fourteen symmetrical and one asymmetrical compounds. Such a variety of structures obtained makes it possible to better evaluate the optical and thermal properties of these substances. 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 length leads to a significant decrease 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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Tuning the charge transfer in organic semiconductor single-crystal interfaces

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Direct contact of two initially insulating organic single crystals can cause significant interfacial electrical conductance and in some cases can even lead to metallic behavior¹. This conductance originates from charge transferred from one material to the other, confined within the first few molecular layers near the interface. The amount of interfacial charge is expected to depend on the electron affinity and ionization potential of the two materials or, equivalently, on the difference in their chemical potentials. However, the detailed microscopic mechanisms responsible for the charge transfer remain to be unexplored. Here we present comparative systematic investigation of high-quality organic single-crystal charge transfer interfaces, formed by Rubrene (tetraphenyltetracene), as donor, and different members of the F_x-TCNQ (fluorinated tetracyanoquinodimethane) family, as acceptors². Through resistivity ρ and Hall Effect measurements we identify the type of carriers that mediate interfacial transport, and determine their density and mobility (see Fig. 1). The measurements have shown that in all interfaces, the charge transfer leads to significantly enhanced interfacial conductivity and that the charge transfer and the conductivity do indeed increase upon increasing the electron affinity of the F_x-TCNQ molecules. In addition to F_x-TCNQ/Rubrene interfaces we have studied F₁₆CoPc(fluorinated Co-phthalocyanine)/Rubrene interface³ which, due to higher electron affinity of F₁₆CoPc molecules compared to F_x-TCNQ, shows even higher charge transfer and electrical conductivity and very well complements the previously obtained results (Fig. 1). All the systematic and consistent results allowed us to develop a simple physical scenario that correctly captures the observed transport properties.

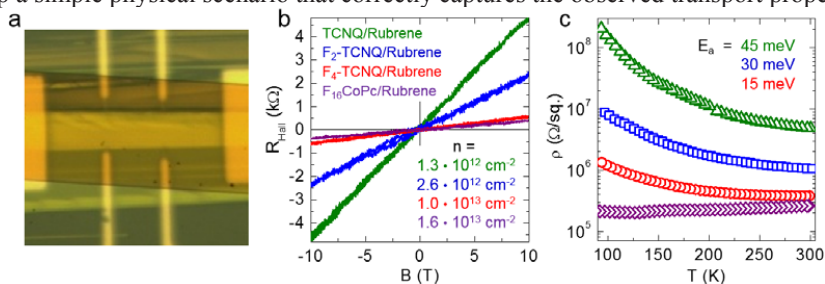


Figure 1. a) Optical microscope image of a representative F₄-TCNQ/Rubrene device. The smaller Rubrene crystal is laminated on top of the bigger F₄-TCNQ crystal with already prepared Au contacts. b) Hall resistance vs. applied magnetic field. From these measurements we have extracted the charge carrier density n and mobility μ ($\mu \sim 1.5 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ for all four interfaces). c) Temperature dependence of the resistivity from which we have extracted the activation energies E_a of the F_x-TCNQ/Rubrene interfaces, while for the F₁₆CoPc/Rubrene interface we observe a decrease of the resistivity with lowering the temperature.

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

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Structure and spin-dependent recombination of charge-separated state in polymer/fullerene composites

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The key process in organic solar cell operation is charge separation under light illumination. When the active layer (typically, the blend of fullerene and conductive polymer) absorbs light, an exciton is formed. It diffuses through the material until it decays to the ground state or reaches the donor-acceptor interface where the electron is transferred from polymer to fullerene. Thus charge-separated (CS) state is formed. Hereafter the CS state evolves into free charges with almost unity quantum yield for many polymer/fullerene blends. Due to the low dielectric constant of organic materials (about 3-4) the Coulomb attraction in CS state is much higher than room temperature thermal energy. The understanding of charge separation mechanism at organic donor/acceptor interface still remains a challenge. To address this problem structure and recombination of the CS state were studied by Q-band pulse EPR spectroscopy (Electron Spin Echo, ESE).

Laser-flash induced echo-detected EPR spectra of the composites of different conjugated polymers with fullerene PC60BM were measured and analyzed. The spectra were obtained using two-pulse microwave sequence $\pi/2 - \tau - \pi - \tau - \text{echo}$ immediately after laser flash with $\lambda = 700 \text{ nm}$ at temperature 40K (delay after laser flash 300 ns). The spectral shape is characteristic for singlet-born spin-correlated radical pair, with some admixture of Emission/Absorption spin polarization¹. It was found that ESE intensity in the middle and on the edges of the spectrum depend differently on microwave intensity. This is caused by relatively strong magnetic interaction (combination of exchange and dipolar interactions) between the spins of the positive and negative polarons constituting CS state which brings the radical pair away from weak spin coupling limit². From this dependence the strength of magnetic interaction 5 MHz was estimated for P3HT/PC60BM composite, which corresponds to interspin distance of about 2 nm. It should be noted that interspin distance distribution is broad for CS state in polymer/fullerene composites³, and the above value corresponds to its lower edge. The feature caused by strong magnetic coupling within CS state dominates the flash-induced EPR spectrum for poor-performing composites MEH-PPV/PC60BM and RRA-P3HT/PC60BM. It is less pronounced for average efficiency composite P3HT/PC60BM and almost disappears for highly efficient composites PTB7/PC60BM and PCDTBT/PC60BM. Thus, the relative amplitude of the „anomalous” EPR feature can be used as a figure of merit for OPV material.

The sign of the „anomalous” feature in flash-induced EPR spectrum of CS state inverts on the timescale of several microseconds at 40K. Presumably this is caused by fast recombination of the CS state in singlet spin state. At longer time triplet CS state with much slower recombination rate dominates the flash-induced EPR spectrum.

This work was supported by RFBR grant № 15-03-07682a.

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Iptycene-based Quinone Molecules: Multi-electron Redox Behaviors and Application in Lithium-Ion Battery Cathodes

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As promising alternative to the conventional transition metal oxide cathode materials for lithium-ion battery, organic redox-active molecules are drawing great attention due to their potential advantages of low-cost, natural abundance, environmental friendliness, and structural diversity. Among others, *p*-benzoquinone (BQ) is one of the simplest π -conjugated organic molecule possessing the lowest molecular weight (MW = 108.10 g/mol) that undergoes reversible reduction with two electrons. The theoretical specific capacity of BQ as electrode-active material is calculated to be as high as 496 mAh/g. However, its high solubility in polar solvents and rather high vapor pressure at room temperature ($P_{\text{BQ}, 25^\circ\text{C}} = 0.1 \text{ mmHg}$) significantly limit its practical use as electrode material in lithium ion batteries.

To solve this issues, several approaches have been proposed such as polymerization of BQ units and/or to synthesize bigger size molecules that contain multiple BQ units. But, these methods inevitably bring about significant decrease of the specific capacity due to increase of redox-inactive weight and suffer from low utilization of redox-active sites as well.

Here, we propose a new molecular design strategy to achieve high specific capacity and energy cathode materials for lithium ion battery using iptycene molecular scaffold. A series of triptycene and pentiptycene derivatives containing multiple BQ units in a rigid tripod structure are synthesized and their redox properties are thoroughly investigated by both theoretical DFT calculation methods and electrochemical analyses. It should be noted that three dimensional arrangements of BQ units of the iptycenes not only facilitate highly reversible access to a large number of redox states but also raise the redox potential. Finally, practical application potential of the iptycenes as cathode materials are evaluated in the 2032-type lithium-ion coin cells. Particularly, an electrode containing a triptycene derivative TT delivers a discharge capacity of 387 mAh/g and an energy density of 1032 Wh/kg, which are one of the highest values among the reported organic cathodes so far, at 0.1 C-rate. It clearly shows two charge/discharge plateaus at 2.6/2.5 V and 3.0/2.9 V, respectively.

Dibenzoindigo: a new nature-inspired semiconductor material for biocompatible organic electronics

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Nowadays a considerable attention is paid to biocompatible and/or biodegradable electronics for various applications including medicine, sensors for social security, environmental monitoring, food industry and etc¹. Most of these applications require non-toxic biocompatible materials. Surprisingly, very little research has been done in order to assess toxicity and biocompatibility of organic semiconductor materials. A natural colorant indigo, which has rather low acute toxicity, demonstrated decent ambipolar semiconductor properties². Theoretical calculations suggested that electrical performance of indigo could be potentially enhanced significantly by extension of the aromatic core of the molecule³. However, in spite of intensive development of this family of organic semiconductors, very few indigoids with an extended π -electron conjugated system are known at the moment.

Here we present a systematic investigation of dibenzoindigo: an indigo derivative with extended π -electron conjugated system. This material shows comparable hole mobilities in organic field-effect transistors with the benchmark semiconductors such as pentacene and DNTT. Relatively easy synthesis of dibenzoindigo, low toxicity and excellent ambient stability in OFETs makes it promising material for designing sustainable and biocompatible organic electronics. Air-stable operation of optical memory elements has been demonstrated using dibenzonindigo as semiconductor and spirooxazine-type photochromic material as a light sensitive component.

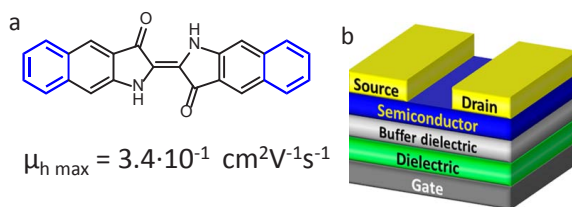


Figure 1. Chemical formula of dibenzoindigo (a) and general layout of the OFET (b)

This work was supported by the Russian Science Foundation (project No. 16-13-10467).

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Environment friendly aqueous processing of [60]fullerene semiconducting films for organic electronics

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Organic electronics is one of the most rapidly progressing fields of science and technology. Inherent properties of organic semiconductor materials allow for fabrication of flexible and even stretchable devices, electronic skin, biostamps, textile-integrated and even implantable electronics. In addition to these exciting functionalities, organic electronics can be made very cheap owing to the application of high throughput roll-to-roll coating and printing techniques.

However, there is a growing concern associated with the environmental impact of the envisioned mass production of organic electronics. On the one hand, typical solvents used for deposition of soluble organic materials are generally rather harmful substances and even their partial release to the atmosphere will result in a serious pollution. On the other hand, using “clean” solvent-free PVD technology is associated with the considerable energy consumption and, thus contributes indirectly to the release of the greenhouse gases to the atmosphere. This challenge can be addressed *via* the development of principally new processing technologies for organic semiconductors allowing for deposition of their thin films from non-harmful solvents such as water and e.g. ethanol.

In this work we present an aqueous processing of fullerene-based organic field-effect transistors (OFETs) using water-soluble C₆₀ derivatives as thermocleavable precursors. We show that sulfur-containing fullerene derivatives undergo facile thermal decomposition above 100°C leading to the pristine fullerene and volatile byproducts as revealed by thermal gravimetry, UV-Vis and FTIR spectroscopy and GPC. This chemistry allowed us to apply water-soluble compounds **1** and **2** (Fig. 1a) for growing thin semiconducting films of C₆₀ using water or water-isopropanol mixtures as environment-friendly solvent systems.

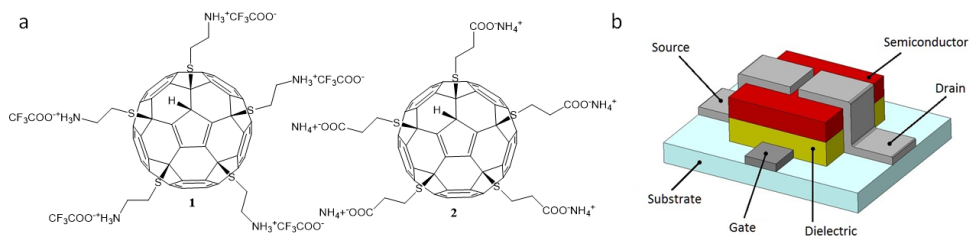


Figure 1. Molecular structures of the water-soluble fullerene derivatives (a) and the architecture of the fabricated OFETs

Top-contact bottom-gate fullerene-based OFETs (Fig.1b) fabricated using thermally annealed films of water-soluble fullerene derivatives **1** and **2** have demonstrated reasonably good electrical characteristics: electron mobility $\mu_e \sim 0.05 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ and current ratio $I_{\text{on}}/I_{\text{off}} \sim 10^4$.

Thus, the presented results can be considered as one of the first successful steps towards the development of sustainable and environment-friendly technologies of organic electronics.

Probing bulk heterojunction morphology of high efficiency organic solar cells by Atomic Layer Deposition

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High efficiency organic solar cells require judicious control of bulk heterojunction (BHJ) morphology. However, characterizing the obtained morphologies so that it can be correlated with processing conditions, is technically complicated. Here we will show how diffusion and retention of organometallic precursors into the different phases can be utilized to spatially map BHJ internal morphology and phase separation.

Generally, Atomic Layer Deposition (ALD) is used to grow metal oxide coatings on functionally terminated surface. When organic nonreactive films are exposed to ALD organometallic precursors, the precursors can diffuse through the free volume, i.e. amorphous and disordered regions, of the film and deposit inside it. Under such conditions, the spatial distribution of the inorganic phase, effectively maps the disordered and amorphous domains of the BHJ.¹

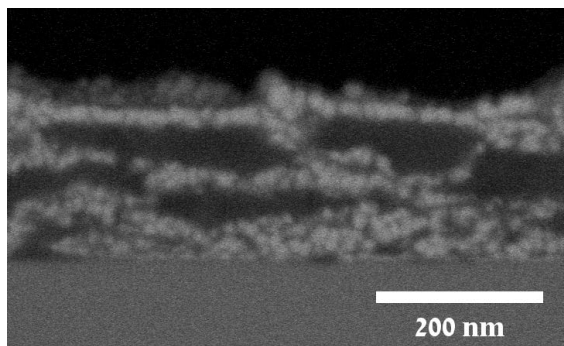


Fig. 1. Cross section BSE HRSEM of PCE11:PC[70]BM BHJ (30:70 wt%) on Si substrate after 80 ALD cycles of DEZ and water at 60°C

Here this methodology is used to characterize high performance BHJs. To do so we selected PCE11, a polymer donor for high efficiency solar cells, and PC[70]BM, a common small molecule acceptor. For example, Fig. 1 shows a back-scattered (BSE) HRSEM cross section image of a PCE11:PC[70]BM BHJ after exposure to 80 ALD sequences of diethyl zinc and water. The bright regions are associated with a polymer-rich phase that retained large amounts of ZnO. This indicates that the polymer phase is sufficiently pure, i.e. with little PC[70]BM, and hence allows significant precursor diffusion through it. In contrast, the film also shows dark regions which are associated with a small molecule-rich phase that does not contain ZnO. We will show that the distribution and size of the different domains depends on BHJ composition and processing conditions allowing us to correlate the morphology and phase separation with the preparation conditions and OPV power conversion efficiency.

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Ambipolar transport in thin layers of new π -conjugated imidazole/carbazole compounds

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Aryl-substituted imidazoles are of perspective photo- and electroactive compounds¹, so push-pull aryl/heteroaryl π -conjugated molecules based on combination of imidazole rings and carbazole or 3,3'-bicarbazole systems (Figure 1) are expected to possess ambipolar carrier transport.

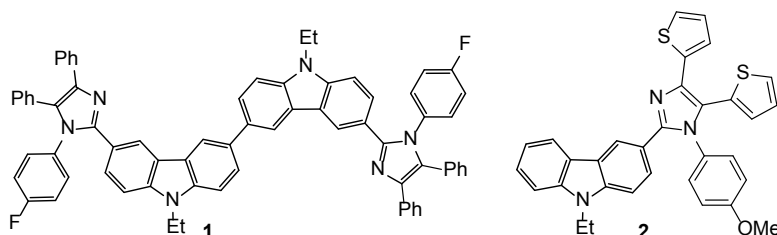


Fig.1. The structure of investigated organic semiconductors **1** and **2**.

In this work, charge carrier mobility in **1** and **2** thermal vacuum-deposited layers was measured by the MIS-CELIV (metal-insulator-semiconductor - charge extraction by linearly increasing voltage) method². Such layers were uniform compared to drop cast layers. In **1**, the mobility values were equal to $5.5 \cdot 10^{-5} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ and $4.5 \cdot 10^{-6} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ for electrons and holes, respectively, and in **2**, they were equal to $3.4 \cdot 10^{-4} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ and $6.2 \cdot 10^{-5} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$, correspondingly.

In the both materials, the mobility of electrons exceeds that of holes. The difference in electron and hole mobility can originate from the arrangement of the molecules in the solid layers which favors for hopping rather electrons over LUMO levels distributed within imidazole moieties than holes over HOMO levels distributed within carbazole systems. The reasons for the better packaging of molecules is thought to originate from the structure of their side chains, the spreader π -conjugation system and small size of the molecules **2** compared to molecules **1**.

For the both organic semiconductores, the method of preparation of a thin layer was found to strongly affect the charge carrier mobility: the mobility in layers prepared from a solution was much lower than that in vacuum-deposited layers³.

This work was supported by the Russian Science Foundation (projects № 16-13-10435 (material synthesis) and 15-13-00170 (charge transport study)).

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Stable organic solar cells based on novel highly soluble star-shaped oligomer

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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 with similar structure. This alkyl-free star-shaped oligomer with electron-withdrawing phenyldicyanovinyl groups possesses a unique combination of extremely high solubility (up to 30 g/L in ODCB) and thermal stability (up to 490 °C) 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:PC₇₀BM/cathode (Ca/Al or PEIE-C₆₀/Ag). These OSC demonstrated a quite good efficiency of 4.5% and good shelf life stability without encapsulation. To optimize the morphology of the active layer, we used various fabrication protocols including thermal and solvent-vapor annealing 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.

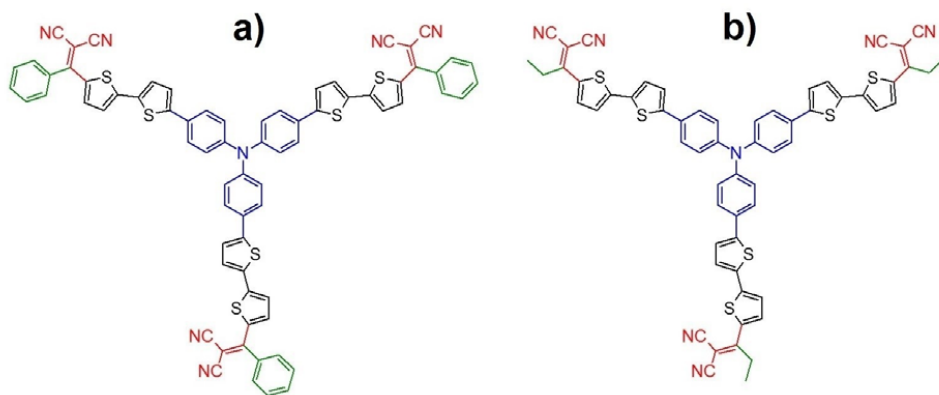


Fig. 1. (a), (b) Structural formulas of SSO N(Ph-2T-DCN-Ph)₃ and N(Ph-2T-DCN-Et)₃.

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

¹ Jie Min, et al. *Advanced Energy Materials*. 2014, 1400816.

The impact of the photoinduced fullerene dimerization vs. generation of stable free radicals on the outdoor operation stability of organic solar cells

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Rapid development of organic photovoltaics (OPV) during the past decade boosted the power conversion efficiency (*PCE*) from poor 2-3% up to practically relevant values of 10-11%.¹ The record efficiencies were demonstrated for bulk heterojunction organic solar cells comprising the fullerene based n-type materials such as [60]PCBM and [70]PCBM. Now it is generally assumed that the photodimerization of [60]PCBM is responsible for the appearance of the “burn in” effect leading to the rapid roll-off in the device efficiency within the first 100 h of operation.² However, it has been shown that [60]PCBM photodimerization can sometimes even enhance the operation stability of organic solar cells, particularly at elevated temperatures, due to the reduction of the fullerene phase mobility suppressing the morphological segregation of the fullerene and polymer components in the active layer.

In this work, we present a systematic study of the outdoor operation stability of organic solar cells based on PCDTBT blends with three fullerene derivatives undergoing different photodegradation pathways. A comparative analysis of the changes in the UV-Vis light absorption and EPR spectra as well as HPLC and GPC profiles of the PCDTBT/fullerene blend samples in parallel with the monitoring the evolution of the photovoltaic performance of the corresponding OPV devices has been carried out. The obtained results allowed us to conclude that the fullerene photodimerization has a negligible effect on the stability of the devices. On the contrary, accumulation of photogenerated free radicals by the fullerene derivatives incorporated in the photoactive layer represents the main device failure mechanism.

This work was supported by the RFBR (grant No. 15-33-20566_mol_a_ved).

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² I. Fraga Domínguez, A. Distler, and L. Lüer, *Adv. Energy Mater.* 2016, 1601320

Surface-enhanced Raman spectroscopy of thiophene-phenylene co-oligomer semiconducting monolayer

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Crystalline organic semiconducting monolayers have high potential for flexible ultrathin electronics. The electrical behavior of devices based on highly crystalline thin films is essentially anisotropic. However, the local monolayer crystalline structure has practically not been studied. To probe the monolayer domain structure Raman microscopy can serve as a useful tool. Due to the Raman anisotropy effect¹, one can distinguish differently oriented domains.

In this work, we report Raman study of semiconducting Hex-TTPPT-Hex monolayer prepared by solution cast-assembly technique.(Fig 1.a) As the monolayers give a very weak Raman signal, to amplify it, we apply surface-enhanced Raman spectroscopy (SERS). For this, we prepared a Si-substrate covered with thin gold film using thermal evaporation. Then a monolayer film was deposited.

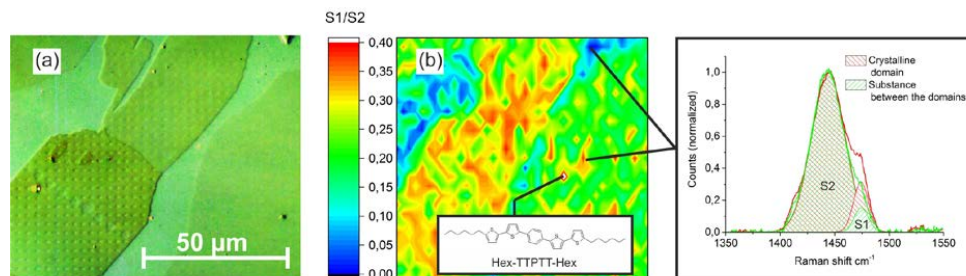


Fig. 1. (a) Microscope image of the monolayer (C-DIC) (b) Raman map of the selected area. We used Red laser (633nm) with a power of 20mW for Raman excitation. S1/S2 area ratio of 1445 cm^{-1} and 1475 cm^{-1} peaks was used for Raman Map calculation.

We succeeded in obtaining Raman map for Hex-TTPPT-Hex. (Fig 1.b) Analyzing this map in accordance with polarized optical(C-DIC) and atomic force microscopies, we found that Hex-TTPPT-Hex film has a domain structure. Furthermore, Raman mapping allowed us to detect the presence of the monolayer molecules between the domains. The spectrum of molecules between the domains differs from the crystalline one, indicating great difference in orientation of molecules in these areas. We suppose that the substance between the domains is amorphous.

Using theoretical quantum chemistry modelling in GAMESS² allowed us to calculate dependence of Raman spectrum on the orientation of the Hex-TTPPT-Hex molecule. With these data, we developed a model relating the experimental spectra and orientation of molecules in different crystalline domains. These results enable us to control 2-D orientation of the crystals and thus electrical conductivity charge transport of the device.

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² M.W.Schmidt, K.K.Baldrige, et al. *J. Comput. Chem.* 1993, **14**, 1347-1363.

Influence of electrode material on contact resistance of organic field-effect transistors

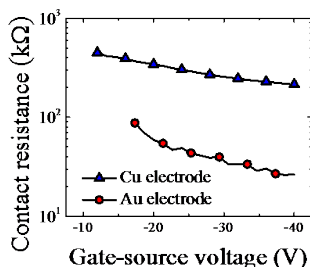
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Since the first organic field-effect transistor (OFET) was successfully demonstrated in 1986¹, it has aroused extensive interest for wide applications in newly booming flexible organic electronics, which are promising in massive fabrication with low cost on large-area rollable substrates². With increasing efforts on the advancement of OFETs, current research focuses on the development of air-stable semiconducting materials with high carrier mobility³ and downscaled short channel devices⁴ to achieve high output current as well as fast switching speed. However, as the channel length becomes shorter, the so-called short channel effect (such as the decrease of effective mobility) becomes prominent, especially for those devices with high carrier mobility, which arises from contact resistance⁵. In particular, the origin of the known gate-voltage-dependent contact resistance is not yet clear, although some models have been tentatively proposed to fit the data.

In the current report, we show voltage dependences of pentacene OFETs with different electrode metals. We propose an electric-field-enhanced thermionic injection model to account for the gate-voltage-dependent contact resistance, which has been commonly observed for OFETs and yet is not well understood. The model is based on the idea of enhanced carrier injection from a metal surface into an organic semiconductor by lowering the injection barrier with an electrostatic field, thus predicting a different dependence of contact resistance on gate voltage in contrast to the conventional simple power function. Detail comparison of proposed model with current crowding model and the resistive network model for electrodes with different injection barrier illustrates capability of each model.



This work was supported by the Slovak Research and Development Agency (grants APVV-14-0739 and APVV-14-0740).

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⁴ Noh Y. Y., Zhao N., Caironi M., *et al.*, *Nat. Nanotechnol.* 2007, **2**, 784.

⁵ Ante F., Kälblein D., Zaki T., *et al.*, *Small* 2012, **8**, 73.

Thin films based on multilayer graphene nanobelts and quantum dots deposited by modified Langmuir-Blodgett technique

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A low-cost and versatile modified Langmuir-Blodgett method was applied here for fabrication of thin flexible photosensitive films based on multilayer graphene (MLG)¹, quantum dots (QDs) and their hybrid structures². These materials can be deposited in thin films onto various substrates, including flexible polymers (like polydimethylsiloxane - PDMS), silicon and glass. This method employs a trapezoidal Teflon® cuvette, where one of the side walls is 45° inclined. First, a low-density suspension containing the nanomaterial (MLG nanobelts or QDs) in a proper solvent is prepared. Then, using a micro-syringe, the suspension is slowly and carefully distributed as a thin layer on the surface of deionized water that fills the cuvette. About 5 -10 minutes after suspension spreading (necessary for solvent evaporation), a film of uniformly distributed MLG or QDs, floating freely on the water surface is formed. The convergence of the nanostructures and the formation of an increasingly compact film is achieved by slowly draining the water through a hole at the cuvette's bottom, thus reducing the water surface area. As the water level drops, the film is transferred onto a vertically oriented hydrophilic substrate placed at the bottom of the cuvette, on the wall opposite to the inclined one. Due to this geometry, the reduced area of the water mirror covered with the compacted film matches exactly to the area of the film deposited onto the substrate, keeping the film density constant during deposition.

Suspensions of MLG flakes and nanobelts (thickness ranging from 3 to 30 nm) in N-methylpyrrolidone (NMP) were used for LB deposition. Uniform thin films were obtained, being possible to have a mean thickness of about 50 – 60 nm for a single LB deposition. The as-fabricated MLG films show sheet resistance from ~10 Ω/sq to ~ 1 MΩ/sq. These changes in resistance can be achieved just by varying MLG concentration in suspension (0.1 – 1 mg/mL), volume of suspension used (60 – 500 µL) and number of depositions (from 1 up to 10). Suspensions of colloidal CdSe/ZnS (core/shell) quantum dots (2.5 nm or 5.3 nm diameter), in toluene or chloroform as solvents, with concentration of ~ 15 µg/mL and volumes in the range of 1 – 15 µL were used for obtaining QDs thin films. AFM analyses were performed to show good QDs film uniformity, with the total thickness reaching 2 – 3 QDs monolayers in a single deposition.

Finally, hybrid structures (QDs over MLG) were fabricated by subsequent depositions of MLG and QDs films. This type of structures can found potential applications in photonics devices³, and the study of optoelectronic properties of so produced hybrid structures is currently in progress.

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Push-coating: a low-cost and green fabrication approach to polymer electronic devices

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Due to both their easy processability and compatibility with roll-to-roll processes, polymer electronics is considered to be the most promising technology for the future generation of low-cost electronic devices such as light-emitting diodes and solar cells. However, the state-of-the-art deposition technique for polymer electronics (spin-coating) generates a high volume of chlorinated solution wastes during the active layer fabrication. Here, we demonstrate that devices with similar or higher performances can be manufactured using the push-coating technique¹ in which a polydimethylsiloxane (PDMS) layer is simply pressed against a very small amount of solution (less than 1 μL) which is then left for drying. By tuning the PDMS thickness, both the applied pressure and the solvent diffusion rates can be optimized to generate the desired active layer thickness. Unlike spin-coating, push-coating is a slow drying process which induces a higher degree of crystallinity in the polymer thin film without the necessity for a post-annealing step. The polymer light-emitting diodes based on poly(9,9-dioctylfluorene-*alt*-benzothiadiazole) (F8BT) and solar cells consisting of poly(3-hexylthiophene):phenyl-C61-butyric acid methyl ester (P3HT:PCBM) prepared by push-coating exhibit slightly higher performances with respect to the reference spin-coated devices while at the same time reducing the amounts of active layer materials and chlorinated solvents by 50 times and over 20 times, respectively. As push-coating is a roll-to-roll compatible method, the results presented here pave the way to low-cost and eco-friendly fabrication of a wide range of emerging devices based on conjugated polymer materials.

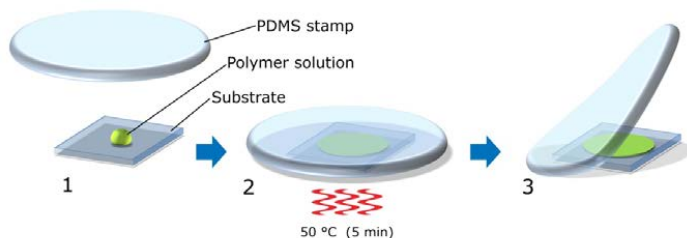


Fig. 1. Schematic representation of the push-coating process.

This work was supported by the scientific cooperation agreement between CNR and RAS (project Giovannella/Khotina).

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Water/alcohol soluble conjugated polymers as electron-injecting layers for OLED technology

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Interfacial engineering has been recently identified as a fundamental strategy for maximizing efficiency and stability of organic electronic devices. To this aim, a new class of water/alcohol-soluble materials comprising a π -conjugated backbone with pendant polar or ionic groups has been recently developed^{1,2}. These polar conjugated polymers have the typical properties of polymeric semiconductors, such as easy processability, chemical tunability, lightness and flexibility, and are suitable for meeting the growing demand for environmentally friendly materials. In fact, the solubility in water and alcohols obtained by the incorporation of polar/ionic side groups can potentially provide increased biocompatibility for sensor applications and more environmentally friendly manufacturing options. Moreover, the possibility for orthogonal solvent processability opens the way to all-solution-processed organic multilayer devices.

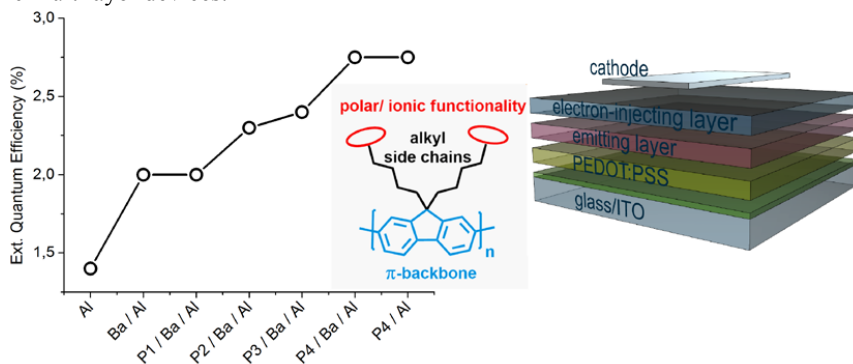


Fig. 1. The external quantum efficiency of the devices with different types of electron-injecting layer/cathode configurations (left); a general structure of the employed polar polymers (center); a scheme of multilayer OLED (right).

In this communication we present the application of polar conjugated polymers featuring a fluorene-based backbone with pendant sulfonate (P1), ammonium (P2), PEGylate (P3) and phosphonate (P4) groups. The polymers have been employed as electron-injecting layers (EIL) in all-solution-processed organic light-emitting diodes (OLEDs). In almost all the cases by using EIL we obtain an improvement of the performance with respect to the reference device with only metallic cathode. For the best case, the diode with only P4/Al cathode exhibits the same external quantum efficiency as the reference device with P4/Ba/Al cathode, proving excellent injecting properties of the polyelectrolyte. OLEDs with the presented polymers pave the way to efficient, fully-solution-processed solid-state light sources.

This work was supported by project Giovannella/Khotina – the scientific cooperation agreement between CNR and Russian Academy of Sciences.

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Controlled Drift of Small Molecule Dopants in Organic Semiconductors

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Stable electrical doping of organic semiconductors is fundamental for the functionality of high performance devices. It is known that small molecule dopants can be subject to diffusion in P3HT. We find that the dopants F₄TCNQ and Mo(tfd-CO₂Me)₃ additionally drift upon application of a voltage above a certain threshold in thin films of doped P3HT. This drift is not observed in the small molecule Spiro-MeOTAD. As a consequence of the dopants' directional movement in P3HT, a dedoped region forms at the negatively biased electrode, increasing the overall resistance of the thin film. In addition to electrical measurements, we use optical microscopy and spatially resolved infrared spectroscopy to prove the drift of dopants and estimate drift mobilities. We show that this controlled drift over a length scale of micrometers is reversible and present a memristive device to illustrate the applicability of this effect. Our study emphasizes the importance of dynamic processes under operating conditions that have to be taken into account even for single doped layers.

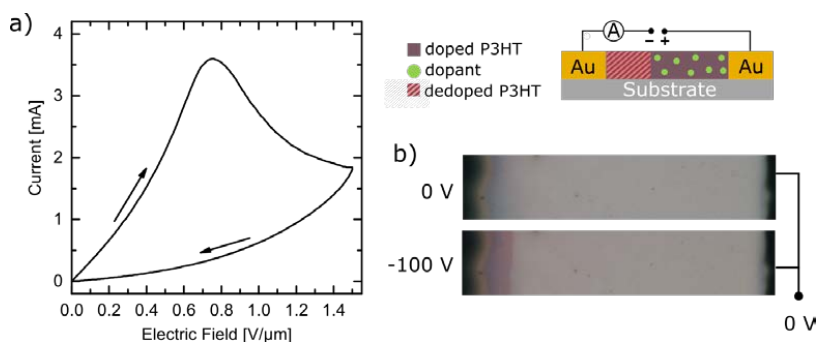


Fig. 1. (a) Current-voltage characteristic of a thin film of P3HT doped with Mo(tfd-CO₂Me)₃ using the layout depicted in the schematic. The current reaches a maximum at a certain threshold electric field and even decreases above, indicating a growing total resistance of the device. (b) Optical micrographs of the channel between two gold electrodes filled with P3HT:F₄TCNQ for electric field strengths of 0 V μm⁻¹ and 0.8 V μm⁻¹. The red area indicates dedoped P3HT.

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Theoretical and experimental study of the capacity fading in lithium-poly(naphthalene diimide) batteries

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Organic redox-active carbonyl-based polymers are intensively explored as promising high-capacity cathode materials for lithium and sodium batteries.¹ In spite of many inspiring reports appeared in the field, practical implementation of this group of materials is restricted severely by their poor operation stability.

In the present report, we address the capacity fading problem in the recently reported lithium-polyimide batteries. We show experimentally that the polyimide NDI-HY cathode degradation becomes less pronounced at high charge/discharge current rates, suggesting the involvement of some intermediate redox species in the degradation process. Replacing a standard liquid electrolyte with the polymer electrolyte entirely suppresses the degradation and results in a stable battery performance over 700 cycles (fig. 1a, curve 4). DFT calculations have revealed that the investigated polyimide undergoes fragmentation to low molecular weight species via rupture of the N-N bonds in the main polymer chain under lithiation (fig. 1b). The solvation of the polymer fragments and their subsequent dissolution results in the battery capacity fading.

The proposed organic cathode degradation mechanism has been proved experimentally using UV-vis spectroscopy and electrospray mass spectrometry, which proved the accumulation of low molecular weight fragments of in the battery electrolyte under cycling.

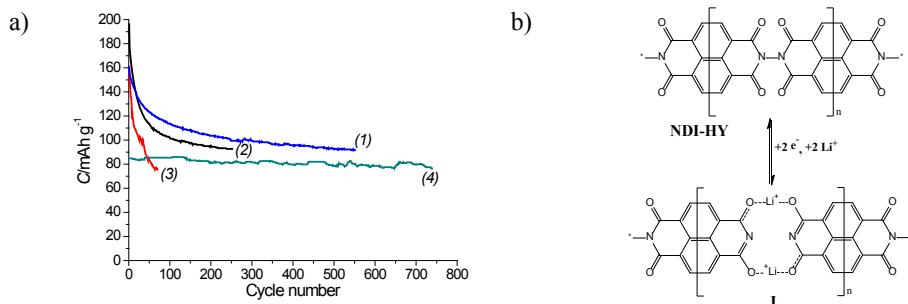


Fig. 1. Cycling performance of the Li-NDI-HY battery with standard liquid electrolyte under different rates: 2C (curve 1); 0.5C (curve 2); 0.1C (curve 3). Curve 4 shows a behavior of the battery with the polymer electrolyte at a 0.5C rate (a). Spontaneous cleavage of the N-N bonds in the NDI-HY backbone under reduction and the formation of coordination polymer I composed of low molecular weight moieties connected by Li⁺ cations (b)

The achieved insight in the electrochemical behavior of the investigated model NDI-HY polyimide structure provides very useful guidelines for designing novel cathode materials with enhanced stability with respect to the electrochemical lithium insertion.

This work was supported by RSF (grant № 16-13-00111).

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Non-fullerene Tetraazaperylene-based Electron Acceptors for Organic Photovoltaics: EPR Measurements

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Polycondensed materials of new kind were synthesized based on chemistry of anthrathiophene and acetylene compounds: 2,8-dialkoxy-1,3,7,9-tetraazaperylene (Fig.1).

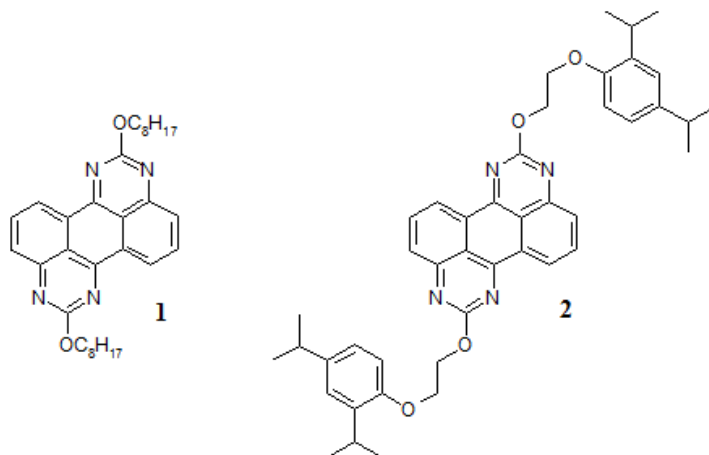


Fig.1. The tetraazaperylene-based compounds **1** and **2**.

The energy values of frontier orbitals were obtained by cyclic voltammetry for both compounds **1** and **2**: $E_{\text{HOMO},1} = -3.51$ eV, $E_{\text{LUMO},1} = -5.69$ eV, $E_{\text{HOMO},2} = -3.53$ eV, $E_{\text{LUMO},2} = -5.79$ eV. Obtained values show that these compounds can be used as electron acceptor in blend with conductive polymer P3HT. The light-induced radicals $\text{P3HT}^+/1^-$ and $\text{P3HT}^+/2^-$ were detected by continuous wave and pulse EPR spectroscopy methods under light illumination. CW EPR signal of 1^- and 2^- were simulated as single line with Gaussian broadening 7.5 G and 7.2 G respectively. The recombination kinetics were obtained by using the CW EPR spectroscopy method. The radicals were found to have lifetime more than 15 minutes and light-induced EPR signal does not reach the value of dark signal after this time at $T = 80$ K.

Obtained data suggests that the tetraazaperylene-based materials are possible alternative small-molecular compounds as an electron acceptor for organic photovoltaics.

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Characterization of naphthalene derivatives with different alkyl side chains

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A significant industrial growth in the area of organic semiconductors over the past few years has been well recognized by the scientific community¹. The advancement is especially noticeable in organic electronic systems such as flexible electronic displays, organic field effect transistors (OFETs) and thin-film organic photovoltaic devices. In spite of numerous advantages to the organic circuits and devices, the efficiency of such systems is yet to be comparable to that of silicon based devices. This necessitates the development of advanced, high-performance organic materials with properties comparable to those of conventional electronics materials². In the last few years, a considerable effort has been directed to the development of organic thin-film transistors due to their potential of being used in organic electronics, particularly in flexible screens and other printed electronic devices.

Polycyclic aromatic hydrocarbons are common used in the design of new organic semiconductors. Naphthalene or anthracene cores ensure semiconducting properties, whereas alkyl side chains provide required solubility. However, only few studies have been conducted into the relationship between cores and alkyl side chains as well as their influence on film morphology and electrical properties. In this report we demonstrate the effect of the alkyl side chain for naphthalene bithiophene core. Although the organic semiconductor core should provide required electrical properties, the side chains strongly affect molecular packing in the solid state. As a result, the design of molecular structure is not trivial and requires more deep understanding of film structure. The organic semiconductor films have been characterized in the OFET device to evaluate free charge mobility and the electrical properties have been correlated with surface morphology. It has been found that shorter alkyl chains result in higher effective mobility and larger average grain size of polycrystalline films. Details comparison provides simple roadmap in the design of organic semiconductors with alkyl side chains.

This work was supported by the Slovak Research and Development Agency (grants APVV-14-0739 and APVV-14-0740).

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² Forrest S.R., *Nature* 2004, **428**, 911.

Effect of substituents in photochromic materials of di(hetaryl)ethene series on electrical characteristics of memory devices based on organic field-effect transistors

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Research interest to the optical memory devices based on light-switchable photochromic organic molecules has been steadily growing during the last several years. However, considering the recent review¹, one can notice that the electrical performance of such materials remains inferior as compared to other types of the state-of-the-art organic memories. In particular, light-induced current modulation (switching coefficient) is generally very low (below 10), while the time required for programming of such devices is too long (ranging from 10 seconds to several minutes). Therefore, there is an obvious need for further exploration of this research field in order to boost the electrical performance of the devices.

Di(hetaryl)ethenes represent one of the most important types of photochromic materials due to a favorable combination of chemical stability, versatility of the molecular design and exciting optical characteristics². Recently, we have applied a di(hetaryl)ethane-based photochromic material as a light-sensitive component for designing photoswitchable organic field-effect transistors (OFETs) and optical memory elements³.

In this report we will discuss results of our systematic study of a series of differently substituted photochromic di(hetaryl)ethenes in OFET-based optical memory elements. The synthesis of six novel compounds of 2-oxazolyl-3-thienyl-cyclopentenone will be presented. We will show that electron-rich and electron-withdrawing substituents in photochromic molecules strongly affect ON/OFF switching coefficients, programming speeds, write-read-erase cycling stability, width of memory windows and retention characteristics of the devices.

The obtained results allowed us to find some fundamental correlations between the chemical structure of the photochromic materials and their electrical performance in photoswitchable OFETs. Eventually, further development of this project might result in a significant progress in the design of OFET-based optical memory elements with the characteristics meeting the pragmatic commercialization benchmarks. There is also a promise to apply the same concept and materials for construction of ultrasensitive photodetectors with high (>1000) signal amplification ratios.

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³ Frolova, L.; Rezvanova, A.; Shirinian, V.; Lvov, A.; Kulikov, A.; Krayushkin, M.; Troshin, P. *Adv. Elec. Mater.* 2016, **2(3)**, 1500219.

Probing the Amorphous Domains in P3HT/Fullerene Blends

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The heart of every organic photovoltaic device (OPV) is the photo-active layer based on an organic donor:acceptor bulk heterojunction (BHJ). Generally, the arrangement and morphology of the BHJ dictate the performance and efficiency of the device. However, controlling the complex structure, composed of both ordered and disordered domains, is a challenging task. Moreover, methods for characterizing the disordered domains are scarce. In this work we demonstrate a novel approach to map and study the disordered domains in BHJs. The BHJs films are introduced into a commercial Atomic Layer Deposition (ALD) system and exposed to a sequence of gas phase precursor pulses. The precursors diffuse preferentially through the amorphous domains and convert sub surface to the respective metal oxide. Consequently, the inorganic phase spatially maps the amorphous domains of the BHJ. The BHJs studied here are blends of the commonly used conjugated polymer donor, P3HT, with various fullerene derivatives i.e., PC₆₀BM, PC₇₀BM, BIS-PCBM and ICBA. ALD-exposing the BHJs with varying fullerene loading and following the selective subsurface deposition of ZnO by optical methods, electron microscopy and EDS quantification, allows us to selectively probe the distribution, amount and composition of the amorphous intermixed phase in the different BHJs and to compare the BHJs with different fullerene derivatives. Interestingly, we find that blends with PC₆₀BM, PC₇₀BM and BIS-PCBM deter ZnO precursor infiltration indicating that these fullerenes quickly occupy the amorphous domains of P3HT significantly reducing the free volume available for precursor diffusion. Additionally, at high fullerene loading, fullerene crystallization prohibits subsurface inorganic deposition altogether. In contrast, blends with ICBA allow subsurface deposition even up to 60 %wt. fullerene. This is due to stronger film vitrification and higher thermodynamic compatibility of the ICBA with P3HT which stalls phase separation during the spin coating process. Moreover, we are able to indirectly follow the vertical distribution of ICBA molecules inside the organic blend and to correlate reported device performance with morphological evolution due to thermal annealing.

Photo- and electroluminescence of metal-organic complexes with zinc and beryllium

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Three decades have passed since the publication of the first light emitting diodes based organic compound 8-hydroxyquinoline aluminum (Alq3) and devices based on OLED are producing in the industrial scale, but the synthesis of new compounds and their investigation is continuing. A number of goals are pursued: a high efficiency of the device, the radiation in the required spectral range, stable performance.

OLEDs currently are manufactured either by using light emitting polymers or small molecules. Polymers are interesting for the opportunity of producing devices using the ink jet printing method. Small molecules are interesting for creating multilayer structures to control the speed of the electrons and holes flow and achieving high brightness performance and efficiency of the device.

Metal complexes are the most promising from the huge set of existing organic phosphors for extracting light in the field of applied voltage. OLEDs based on iridium complexes, osmium, platinum are one of the most highly effective, but the precursors are very expensive for the mass production of devices. Particularly for this reason the search for compounds based on metals such as zinc and beryllium continues. In the compounds of this class metal plays mostly a coordinating role, and all photophysical processes are played in the ligands. This provides great possibilities of varying the emission area and the device efficiency.

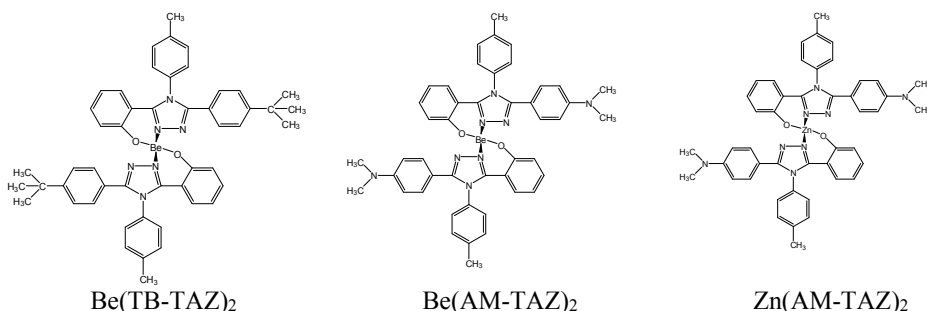


Fig.1. Structure of compounds

In this paper we investigated metal-organic complexes with zinc and beryllium (Zn[AM-TAZ]₂, Be[TB-TAZ]₂ and the Be[AM-TAZ]₂). Photoluminescence characteristics were studied in solutions and films. Analysis of the spectral properties of complexes indicates that the complex itself, undisturbed by intermolecular interactions, the radiation corresponds that lies in the area of ~ 400 nm irrespective of the nature of the ligand and metal. OLED-structures were established on the basis of these compounds. The greatest emission intensity ~ 1000 cd / m² provides Be(AM-TAZ)₂. Be(AM-TAZ)₂ and Zn(AM-TAZ)₂ with different metal, have different intensity of brightness and spectral characteristics. The spectral characteristics of electrical and photoluminescence OLED-structures coincide.

The work is performed in the framework of the grant № 15-12-00034 of Russian Science Foundation.

Characterization of organic-based devices by ToF-SIMS depth profiling

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Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a very effective tool to probe chemical composition throughout the bulk of the device at any stage of its life cycle¹⁻³. Particularly, stability, reproducibility and degradation issues can be addressed through accurate ToF-SIMS depth profiling^{1,2}. Despite some of the side-effects associated with SIMS sputtering of the multilayer samples¹, depth profiles are increasingly used in discussion of such important processes as diffusion of admixtures or interaction of adjacent layers².

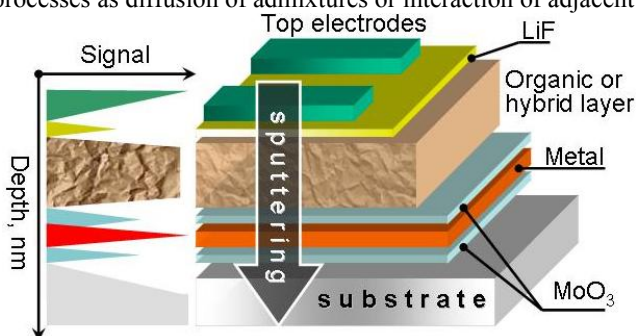


Fig. 1. Schematic of samples and measurement procedure.

In this report we present our results on the ToF-SIMS analysis of the photovoltaic devices obtained by sequential or co-deposition of organic/inorganic layers by vacuum techniques. Bottom electrodes in such devices were transparent conductive thin-film composites of ‘Oxide/Metal/Oxide’ type³ (Fig. 1). Phthalocyanines, fullerenes or hybrids were used as photoactive layers, and a LiF buffer was inserted between the photoactive layer and the top evaporated metallic electrode (Fig. 1). Thus fabricated devices were studied with a TOF.SIMS5 instrument in a dual-beam regime. Probing and sputtering conditions were carefully optimized to achieve the depth resolution of ~ 1 nm³. The mass spectra were measured in the range of 1-1100 a.m.u. in both positive and negative secondary ion mode. From these, practically important elements (ions), ionic clusters, molecular fragments and, if possible, whole molecular ions were selected, and their absolute yields were analyzed as a function of sputtering time.

Photoelectrical characteristics of devices were measured and compared with the data provided by ToF-SIMS depth profiling (and by other methods like XRD, microscopy, spectroscopy). The experimental results are interpreted in terms of diffusion of atoms or sometimes polyatomic species in the depth of the device depending on the permeability of interfaces. Both upward and downward diffusion^{1,3} was revealed, which causes changes in the chemical structure of layers (or interfaces), and hence in their functionality.

This work was supported by RFBR (projects № 15-08-06364, №15-02-02947).

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Red light-emitting polynorbornenes with cyclometaled iridium(III) complexes, carbazole and organosilicon groups in side chains

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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- and triarylsilicon-containing comonomers via Ring-Opening Metathesis Polymerization. The formed polymeric products (Fig. 1) revealed an intense photoluminescence (PL) and electroluminescence (EL) of red color.

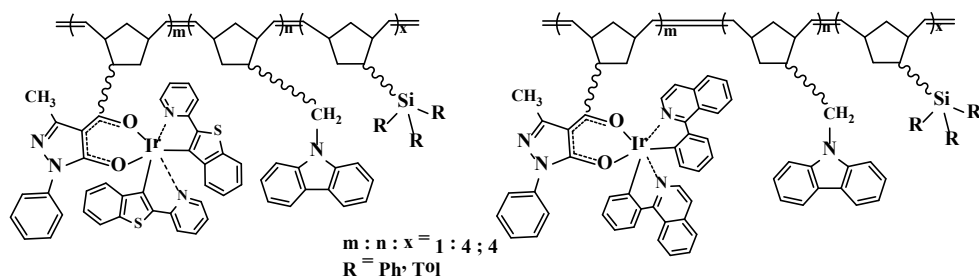


Fig. 1. The synthesized iridium-containing copolymers.

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 and organosilicon groups was observed. Model OLED devices based on iridium polymeric emitters - ITO/Ir-polymer/BATH/Alq₃/Yb showed maximum brightness up to 1648 cd/m², maximum current efficiency – 3.13 cd/A, maximum power efficiency – 0.98 lm/w.

This 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).

Novel organosilicon derivatives of [1]benzothieno[3,2-b][1]-benzothiophene: synthesis and semiconductor properties

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Nowadays one of the perspective directions of organic electronics is design and synthesis of novel organic semiconducting materials for organic electronic devices such as organic light emitting diodes¹ (OLEDs), organic photovoltaics² (OPVs) and organic field-effect transistors³ (OFETs), including self-assembled monolayer field-effect transistors⁴ (SAMFETs). Today these devices are among the most promising, since charge transport in OFET occurs mainly in one or two molecular layers of the organic semiconductor adjacent to the dielectric⁵. Ones of the most efficient OFETs are based on [1]benzothieno[3,2-B][1]-benzothiophene (BTBT) due to its high charge carrier mobility and stability of the molecules⁶. Recently we elaborated a novel fast, easily processible and highly reproducible approach to SAMFETs fabrication by Langmuir technique. For this purpose, tetramethyldisiloxane dimers with aliphatic spacers between the siloxane core and conjugated fragment were used. Such molecules were proved as promising semiconductor material for the fabrication of SAMFETs by Langmuir techniques⁷. In this work we decided to synthesize a number of new dimers with different length of the aliphatic spacer (C6, C7, C11⁸) and BTBT as a conjugated core (Fig.1). The synthesis was carried out using Grignard reaction, Friedel–Crafts acylation and hydrosilylation reactions. The structure and purity of all intermediate and final compounds were confirmed by HPLC, ¹H-, ¹³C-, ²⁹Si-NMR spectroscopy, as well as elemental analysis.

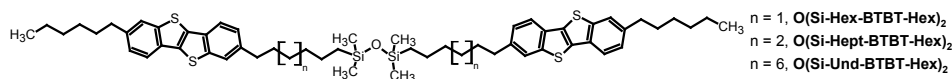


Fig. 1. Structural formula of synthesized and investigated molecules.

Semiconducting properties of the new materials were investigated in the monolayer OFETs fabricated by Langmuir-Schaeffer (LS) technique. All the dimers showed Langmuir isotherms and Brewster micrographs typical for crystalline films. LS semiconducting monolayers reveal similar morphology not depending on the length of the aliphatic spacer of the molecule. Fully covered highly-ordered monolayers with vertical orientation of BTBT fragments having small amount of holes and separate regions of bilayer were demonstrated. The largest saturated hole mobility ($2 \times 10^{-2} \text{ cm}^2/\text{Vs}$) was obtained for the SAMFET based on **O(Si-Hept-BTBT-Hex)₂**. Thus, this LS SAMFET showed excellent semiconducting properties for solution-processed self-assembly.

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

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Crystals of organic conjugated rod-like co-oligomers: structure and peculiarities of growth from solutions

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The most attractive ways of organic crystals growing for the optoelectronics are the methods of growth from solution from the standpoint of simplicity of execution and cheapness. However during the crystallization of organic substances with a spatially extended molecule (spherical, disc-shaped, rod, etc.) one can often observe a substantial anisotropy of growth that may lead to certain difficulties in obtaining of the required size and orientation crystals. This report is devoted to analysis of relationship between the crystal lattice type and way of packing of conjugated rod-like co-oligomers on the one hand and the characteristics of crystal growth from solutions on the other hand. The co-oligomers of this kind can be divided into two groups depending on the nature of the crystal habit formation. During the growth process the co-oligomers of first group tends to the formation of a flat crystals in the form of thin films or plates (fig. 1a,c) with monoclinic lattice and molecular packing in form of parallel herringbone layers oriented along the (001) direction (fig. 1e) [1,2]. Another group of co-oligomers, as a rule, is characterized at crystallization by the formation of needle-like or rod-like crystals (fig. 1b,d) with a triclinic lattice type and packing of the molecules in the form of brickwork (fig. 1f). The report also discusses the influence of the molecular structure factor, crystal lattice defects and environmental conditions on the kinetic and thermodynamic characteristics of crystals growth.

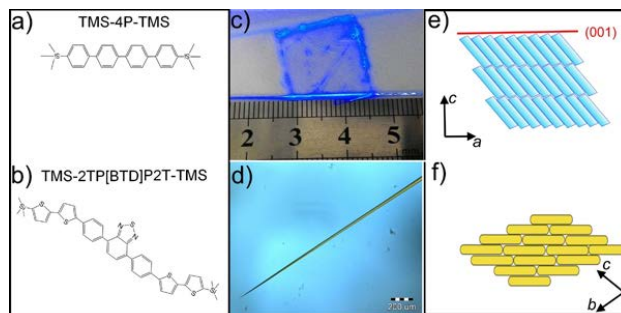


Fig.1. a) and b) – chemical structural formulas and abbreviation of novel rod-like co-oligomers; c) – optical image of TMS-4P-TMS single crystal film; d) - optical micro-image of TMS-2TP[BTD]P2T-TMS needle-shape single crystal; e), f) – schematic illustration of crystal packing ways.

This work is supported by Russian Foundation for Basic Research (project 16-02-00931-a).¹

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A Significant Improvement of Dye-Sensitized Solar Cell (DSSC) Performance by Donor Substitutions on the π -Linker of D- π -A Organic Dye

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Dye-sensitized solar cells (DSSCs) have been intensively investigated since the report of highly efficient ruthenium complex-sensitized TiO₂ solar cells by the Swiss scientists. Currently, the highest overall conversion efficiencies were achieved from the Ru complexes and zinc porphyrins-sensitized cells. However, pure organic dyes exhibit not only higher extinction coefficient, but simple preparation and purification procedure with a low cost. Lately, enormous progress has been made in this field and the highest overall photoelectric conversion efficiency of solar cells sensitized by organic dyes containing an electron donor (D) and an electron acceptor (A), separated by a π -conjugation bridge (π) has reached the level of inorganic dyes. This indicates the promising perspective of metal-free organic dyes. In this presentation, we will report on the first detailed study on the effect of donor substitutions on the π -linker of the basic D- π -A organic dyes aiming to improve the performance of organic dye for DSSCs. A series of new molecularly engineered D- π -A dyes, comprising triphenylamine (TPA) as a donor, terthiophene containing different numbers of TPA substitutions as a π -conjugated linker and cyanoacrylic acid as an acceptor was synthesized and characterized. The effect of different dye structures on the performance of the DSSCs was investigated systematically with theoretical, photophysical, photovoltaic as well as photoelectrochemical methods and compared with the traditional D- π -A dye. The introduction of electron donating TPA substitutions on the π -linker of D- π -A dye benefited on a decrease of the electron recombination between redox electrolyte and the TiO₂ surface as well as an increase of the electron correction efficiency, leading to improved open-circuit voltage (V_{OC}) and short-circuit current (J_{SC}). Consequently, DSSC sensitized by the new dye bearing two TPA substitutions on the terminal thiophene ring of the π -linker delivered the best power conversion efficiency, reaching 8.08% at AM 1.5 simulated sunlight, a remarkable improvement of about 41% compared with the simple D- π -A dye reference cells' 5.72%, owing to its high J_{SC} and V_{OC} . With the addition of CDCA as a coadsorbent, the best performing cell exhibited an impressive conversion efficiency of 9.02% (J_{SC} = 16.91 mA cm⁻², V_{OC} = 754 mV, FF = 0.705), exceeding that of the N719-based standard cell (8.20%).

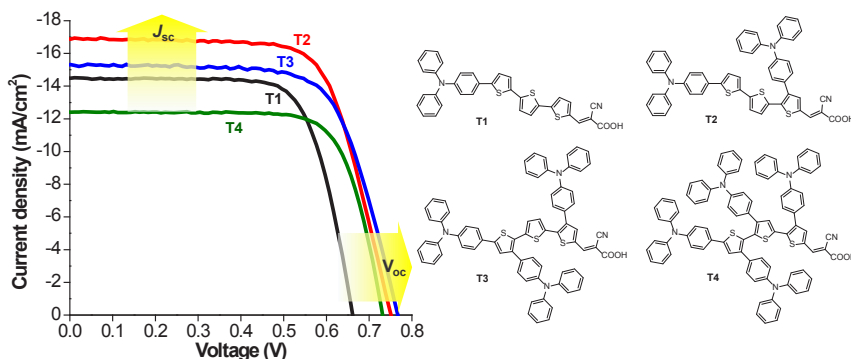


Fig. 1 I-V plots of the DCCSs and molecular structures of the dyes

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A step-by-step theoretical study of monomers for all-conjugated block-copolymers

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Conjugated polymers are promising materials for application in organic electronics due to their low cost, easy processing from solution and flexibility. Advanced technologies need both simultaneous n- and p-type conductance, i. e. ambipolarity, and this can be realized, for instance, combining benzothiadiazole (BTZ) and diketopyrrolopyrrole (DPP) [2]. We have investigated two monomers for further application as block-copolymer using DFT methodology. First we evaluated their elementary consisting units, namely BTZ and DPP flanked with furan (*Fu*) or thiophene (*Th*) rings and further their monomers (Fig. 1). We have compared their conformational, electronic, optical and charge transport properties. Additionally, the binding energies of isolated dimers with different spatial orientation of monomers were calculated in order to describe the π - π interactions within segregated or mixed stacks.

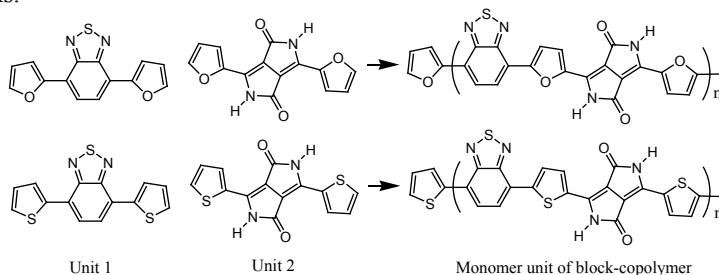


Fig. 1. Structural formulas of the six molecules under investigation: with *Fu* flanks (top) and with *Th* flanks (bottom).

We found out that the energy differences between the *cis* and *trans* conformers and the rotational barriers for the flanks in the units are much lower for the compounds with *Th* π -bridges as compared to *Fu*-containing molecules, but the electronic and optical properties remain the same [1]. The predicted π - π distances in isolated stacks of monomers coincide with the corresponding distances obtained from the individual units in the case when the molecules are oriented face-to-face. The reorganization energies and the electronic couplings are calculated in order to obtain the charge transport properties according to semiclassical Marcus theory. Thiophene derivatives demonstrate higher charge transport mobilities in almost all the simulated systems [3]. The results of the study are compared with available experimental data [2].

This work is funded by the European Union (ERDF) and Free State of Saxony via ESF project 100231947 (Young Investigators Group "Computer Simulation for Material Design - CoSiMa).

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Indolo[3,2-b]indole as a new electron donor for efficient thermally activated delayed fluorescence (TADF) emitters in organic light-emitting diodes (OLEDs)

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Thermally activated delayed fluorescence (TADF) mechanism is drawing tremendous attention in the field of organic light emitting diodes (OLEDs) because it manifests internal quantum efficiency (IQE) up to 100% through the reverse intersystem crossing (RISC). Theoretically, RISC efficiently occurs when energy difference (ΔE_{ST}) between the first singlet (S_1) and triplet (T_1) states is small enough. To ensure this small ΔE_{ST} , highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) should be properly separated and localized, because ΔE_{ST} has a close relation with degree of wavefunction overlap between HOMO and LUMO. As one of the promising approaches to realize TADF, intramolecular charge transfer (ICT) mechanism is most widely employed with bulky electron donor and/or acceptor units which naturally generate distortion of molecular structure to separate the HOMO and LUMO. In this regard, various combinations of electron donor and acceptor moieties have been extensively investigated to realize highly efficient TADF OLED. Although a lot of electron acceptors for TADF emitters have been developed to date, electron donors are still rather limited to only a few heteroaromatic derivatives including carbazole, dimethylacridine, and phenoxazine.

In this work, we employ indolo[3,2-b]indole (IDID) unit as a new electron donor moiety for TADF emitters. A series of IDID-based TADF emitters, which possess various electron acceptors including cyano (CN-IDID), sulfone (DPS-IDID), benzophenone (BP-IDID), and triazole (Tria-IDID) are systematically designed and synthesized. With increasing ICT strength, S_1 level is decreased while T_1 level is pinned. As a result, ΔE_{ST} in IDID derivatives is minimized to give delayed fluorescence. Particularly, an OLED using Tria-IDID as an emitter shows the maximum external quantum efficiency (EQE_{max}) over 15%, which unambiguously demonstrates the high potential of IDID as an electron donor for TADF emitters.

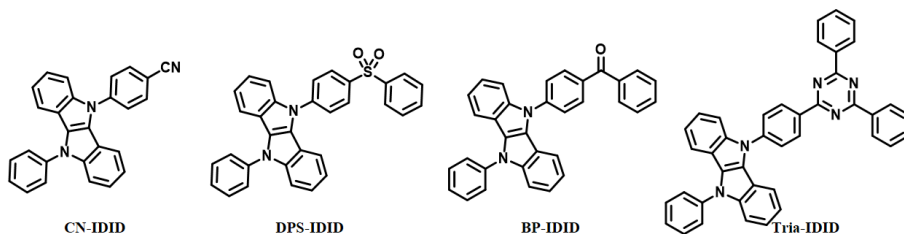


Figure 1. Molecular structure of IDID based target materials

Analytic Modelling of Field Dependence of Charge Mobility in Organic Materials with Correlated Disorder

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Understanding of charge carrier transport phenomena in disordered organic materials is a matter of great interest, since it allows the optimization of electronic devices such as OLEDs, OFETs, etc. The description of transport processes in such materials is a complicated problem, since, unlike inorganics, transport occurs via the phonon-assisted tunnel hopping of charge carriers between energetically disordered localized states. Multiple trapping (MT) model¹ is successfully used, with some restrictions, in order to describe the transport on the base of transport level concept² within the Gaussian disorder model³, providing that energetic correlations of localized states are absent.

However, it is the energetic correlations that yield experimentally observed Pool-Frenkel field dependence of mobility of charge carriers ($\ln \mu \propto \sqrt{F}$). It was shown within dipolar glass model⁴, that deep states, controlling the mobility, are surrounded by a potential well, and the release of a carrier from these states appears to be a multi-step process, involving drift and diffusion motion inside this “quasi-Coulomb” well. A carrier should overcome an energy barrier, formed by the quasi-Coulomb and external field F , which decreases the barrier. In this work, an analytic model of temperature and field dependence of mobility in the framework of dipolar glass model is developed. Mobility is inversely proportional to the energy-averaged reciprocal escape frequency. The escape frequency is expressed as the product of the “attempt to escape frequency” ν , i.e. frequency of jumps from initial state with energy E_i to the nearest state with the same energy at a distance $r_0 = \alpha a_0$, and the probability for a carrier to escape from a potential well, η . The probability η is calculated according to Onsager model. If the field F is small, $\eta(E_i) = \exp[-(E_c - E_i)/kT]$. The term E_c quantifies reduction of an energetic barrier below the average energy. Practically it is a transport level, since energetic correlations with initial state are weak at the edge of the well. Transport level is used as an analog of mobility edge, which separates extended and localized states (traps) in MT model. The results of this work show, that transport level concept, as well as MT-formalism, can be applied for organic materials with both non-correlated and correlated disorder, at least for the small-field limit, if the states within the quasi-Coulomb well (in the latter case) are considered as a “collective trap”. The model gives the temperature and field dependence of mobility in good agreement with the results of Monte-Carlo modelling within the dipolar glass model^{iv}. Presented approach could also be applied in order to calculate the concentration dependence of mobility using the model with microscopic Coulomb interactions, developed earlier by the authors.

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Nonradiative energy transfer in multilayer Langmuir-Blodgett films based on fluorophores of different chemical structure

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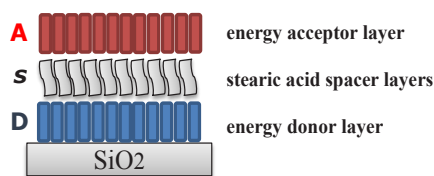
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As we have shown previously¹ for multilayered Langmuir-Blodgett films (LBF) based on naphthalimide derivatives, spatial separation of donor and acceptor layers by ultrathin inert spacer can lead to increase of Förster resonance energy transfer (FRET) efficiency. And the dependence of FRET efficiency in such system on the distance between fluorophore layers has a maximum circa 7 nm. Such behavior of the system can be associated with similarity of the chemical and electronic structures of the studied fluorophores and their identical orientation in the monolayers.

The aim of the present work is to elucidate the effects of similarity of chemical composition of the donor-acceptor couple on the nature of FRET efficiency dependence on the extent of spatial separation of donor and acceptor in 2D system. In order to accomplish this task we studied photophysical properties of the system formed according to the same principle as in our previous study (scheme), but based on fluorophores of different chemical classes: amphiphilic pyrene derivative (PBA - donor) and functionalized hemicyanine dye (HC - acceptor). This couple fits the requirement of high degree of overlap of donor emission spectrum and acceptor absorbance spectrum. We chose stearic acid as an inert spacing layer material, which is a classic surfactant and does not have any absorbance nor emission in the visible light range. The comparison of FRET efficiency in the described systems reasonably was done using acceptor fluorescence excitation (576 nm) spectra. Analysis of the excitation spectra of multilayer films shows that maximum FRET efficiency is observed upon separation of donor and acceptor monolayers by one layer of stearic acid, which corresponds to roughly 2.3 nm. And the FRET efficiency for such system is 1.2 times larger than for the film without spacer interlayer. Further spatial separation leads to sharp decrease of energy transfer efficiency, which is quite explicable in the framework of classical concepts of FRET process.



Thus, it is demonstrated for multilayer systems, in which monolayers of donor and acceptor fluorophores of different chemical structure are separated by an inert layer of varied thickness, that dependence of efficiency of nonradiative energy transfer on the distance between planar components of donor-acceptor couple has a maximum at a finite nonzero thickness of the separating layer.

The study was supported by RFBR grants no. 16-03-00538, 16-29-05284 and 16-33-60024.

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Synthesis, optical and electrochemical study of new bipolar heterocyclic systems, including 1,2,4-oxadiazole moiety

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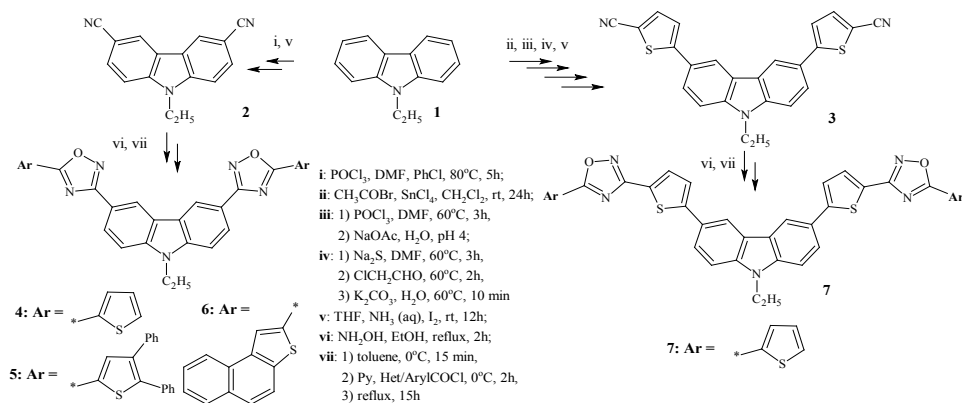
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Nowadays, the interest of the scientists working in synthetic organic chemistry, is increasingly aimed at the creation of materials for organic electronics. Among other tasks this field of organic chemistry includes the elaboration of a design strategy for bipolar conjugated structures as the base of the host-materials used for PhOLEDs. The host materials for highly efficient devices should meet some basic requirements among which are high triplet energy (T1) that prevents energy back-transfer from the guest to the host material (> 2.8 eV for blue PhOLEDs and 2.2-2.8 eV for red and green ones); possession of both types of conductivity (*n* and *p*) that is necessary to reach a charge balance in the light-emitting layer; high morphological stability (high glass transition temperature)¹. In continuation of our previous studies² we have prepared some new bipolar structures embedding 9-alkylcarbazole fragments substituted at the electroactive 3- and 6-positions – an approach which allows to prevent dimerization of oxidized radical-cationic states and to obtain electrochemically stable host-materials. At the same time the prepared structures include 1,2,4-oxadiazole moieties having good electron-transport properties. Additionally, incorporation of this heterocycle enables the distortion of a conjugated chain which, in turn, increases the values of triplet energy³. With the same aim, we have incorporated phenyl groups into the C4 and C5 positions of terminal thiophene units. We found it interesting to prepare bipolar structures embedding electron excessive naptho[2,1-b]thiophene fragments; this type of bipolar compounds have been not yet described.



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Spontaneously generated interlayers in direct and inverted OPVs with silver and gold contacts

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Incorporating interlayers at the organic/electrode interface in organic photovoltaic (OPV) devices has a significant contribution to their efficiency and ambient stability. Recently, spontaneously segregated interlayers have attracted great interest due to their processing simplicity and compatibility with printing methods. Here we will demonstrate that the evaporation of the top metal contact induces a chemical interaction between additives blended in the active layer generating their migration towards the metal/organic interface to form an interlayer. This driving force for segregation can overcome the tendency of high surface energy additives to migrate away from the film surface, and may be suitably applied to a variety of top electrodes. We will focus in this presentation on ambient stable contacts, silver and gold, and P3HT:PCBM blends as a platform for investigating devices with self-generated thiol-based interlayer. X-ray photoelectron spectroscopy (XPS) confirms the selective migration of the additives towards the organic/contact interface and Ultraviolet photoelectron spectroscopy (UPS) shows a sequential modification of the contact's effective work function at the interface. We will show that the modified work function of the contact could be used for both direct and inverted photovoltaic devices. Finally, we will demonstrate the contribution of the spontaneously generated interlayers for high performance blends and ambient stability of unencapsulated OPV devices.

Toward solution processed magnetic nanoparticles for non-volatile memory applications

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Iron oxide nanoparticles (IONPs) are among the most promising candidates for nano-scale magnetic memory applications due to their excellent magnetic properties^{1,2}. The information can be stored depending on the magnetization of the particles. The general drawback of IONPs however is the lack of ferromagnetism in IONPs at room temperature. To overcome this issue, doping of IONPs with cobalt is suggested³. The concentration of cobalt within the spinel ferrite nano crystals also has a significant effect on their magnetic properties. In this contribution we present a systematic study of Co doped IONPs using heat-up synthesis methods (thermal decompositions), wherein different synthesis parameters are surveyed and their effect on the particle size and magnetic properties are investigated. The synthesis was optimized to obtain sub-20 nm highly crystalline and monodisperse ferromagnetic nanoparticles with optimum magnetization and coercivity values (Figure 1). The particles were further modified by grafting polymerization from the surface of nanoparticles. Polymeric shells of different molecular weight are obtained, which allowed well dispersion of the ferromagnetic nanoparticles in common organic solvents. Nanoparticles can be solution processed to form a ferromagnetic thin-film. Solution processable magnetic films can open a new avenue in the low-cost non-volatile memory application.

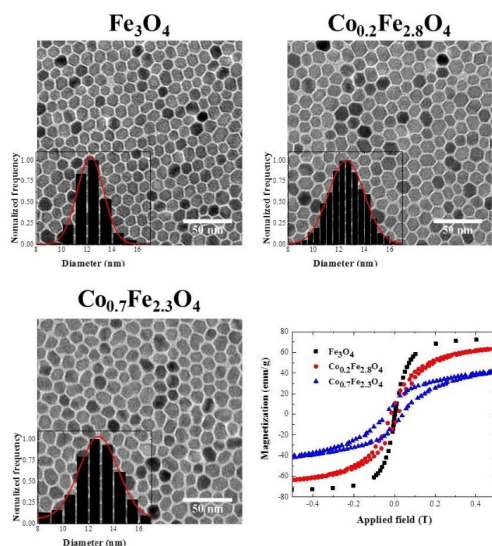


Fig. 1. TEM images of samples with different ratio of cobalt (a) Fe₃O₄, (b) Co_{0.2}Fe_{2.8}O₄ and (c) Co_{0.7}Fe_{2.3}O₄. Particle size distributions obtained by fitting TEM histograms are shown in the insets of the images. (d) Hysteresis loops of all samples at room temperature.

This work was supported by humboldt foundation.

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Ambient Processing of P(VDF-TrFE) Ferroelectric Thin-Films for Application in non-Volatile Memory Devices

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The most commonly used ferroelectric polymer for memory applications is the random copolymer of vinylidenedifluoride with trifluoroethylene (P(VDF-TrFE)). Solution processing of P(VDF-TrFE) at ambient condition (room temperature and relative humidity of 50%) produces rough and unpacked film due to presence of water and vapor-induced phase separation (VIPS); A process well-documented for the fabrication of PVDF membranes. In the absence of water no phase separation occurs and the films are smooth and dense¹.

Moreover, in contrast to inorganic ferroelectrics P(VDF-TrFE) typically shows low remanent polarization. It has been shown that blending P(VDF-TrFE) with nanoparticles (NPs) enhances the polarization². Due to VIPS however, functional capacitors have only been demonstrated for very thick films namely >30 μm with coercive voltage that amount to several kilo volt which is prohibitive for any application.

Here, we first calculated approximate ternary phase diagrams for P(VDF-TrFE)/water/solvent systems, involving solvent evaporation, water condensation, and phase dynamics. We show that the hydrophilicity of the organic solvent is a deciding factor as it determines the ingress rate of water from the ambient into the solution and determines the final morphology. The simulations render morphological features qualitatively consistent with the structures experimentally observed for the rough polymer films. We show that VIPS is effectively hindered by using a solvent that is immiscible with water, and develop an ambient compatible processing recipe for P(VDF-TrFE) with a large processing window. Transparent, closely packed smooth thin-films were obtained under ambient conditions. The yield of functional ferroelectric capacitors with sub-10V coercive voltages was close to unity (>95%).

In the next step, highly monodispersed sub-20 nm NPs were synthesized and blended with P(VDF-TrFE) at different loadings. We show that remanent polarization increases for loadings below 10wt%. The capacitors function at sub-10V with a high functional device yield. Enhancement of remanent polarization can positively influence integration of thin P(VDF-TrFE) films in non-volatile memory devices.

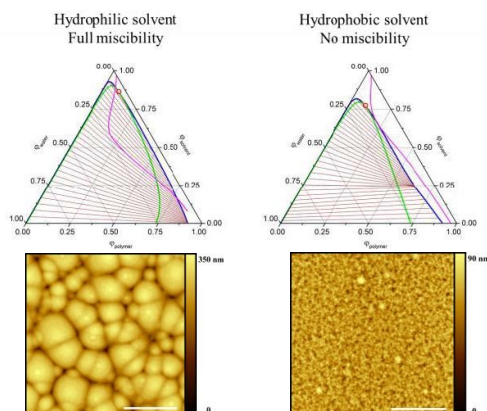


Fig. 1. Calculated ternary phase diagrams for P(VDF-TrFE)/water/solvent systems for both hydrophilic and hydrophobic solvents (top), and the corresponding morphologies experimentally obtained (bottom) with AFM. Scale bar is 10 μm .

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Planar thin-film memristors based on polyaniline and polyethylene oxide

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Non-volatile electronic elements with a resistance determined by the leaked charge history – memristors – could be prepared by the planar thin-film technology¹. In this case the thin-film organic memristor is based on polyaniline (emeraldine salt) and silver chloride electrode separated by polyethylene oxide doped with lithium ions. Functionality of such memristors is caused by electrochemical control of oxidation state of polyaniline film.

In this work the planar thin-film organic memristor (fig. 1) was prepared by sequential deposition of titanium electrodes (2), polyaniline film (3), kapton film (4), a layer of polyethylene oxide doped with lithium perchlorate (5) and silver chloride electrode (6) onto the glass substrate (1). The titanium and silver electrodes were deposited thermally. The polyaniline Langmuir film was transferred onto the substrate by the Langmuir-Schaefer method. Thin polyaniline films for organic memristors may also be prepared by spin coating². The polyethylene oxide layer was placed commonly from water solution onto the polyaniline layer surface and was dried on air. But we could not control the thickness and morphology of the film and the lithium ions quantity.

We have investigated the thickness and conductivity of spin-coated polyethylene oxide film depending on the concentration of the polymer and lithium perchlorate in the solution, duration and speed of the rotation. The resistance of polyaniline and polyethylene oxide thin films and the current-voltage characteristics of the memristors based on such materials have been measured.

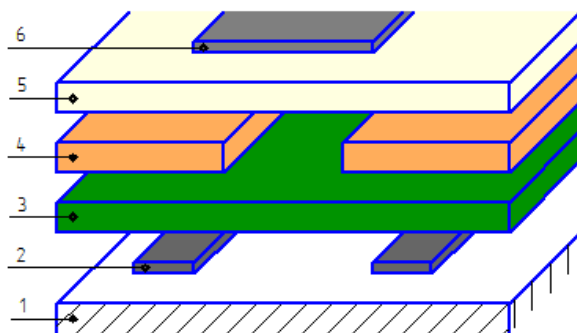


Fig. 1. Schematic construction of thin-film organic memristor (see comments in the text).

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Sorption and Desorption Processes of Toxic Gases and Water Vapour in Monolayer Langmuir-Schaefer Organic Field-Effect Transistors

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In recent years, organic field effect transistors (OFETs) have been studied as a basis for the low-cost sensor technology¹ with a perspective to be fabricated by exclusively solution processing. The sensitivity of such devices significantly depends on the semiconductor thickness since the adsorbed analyte molecules modulate the charge transport in OFET by electrostatic interactions, which have a strong distance dependence. Downscaling the thickness of the active layer to a 1-2 molecular layers therefore promises that the ultrasensitive gas sensors could be obtained using OFETs (Fig. 1a). Indeed, the monolayer sensors based on self-assembled monolayer field-effect transistors (SAMFETs) demonstrated very high sensitivity to NO (down to ppb level).² However, the purposed approach involved a long (15 hours) semiconductor deposition process, which could hardly be upscaled.

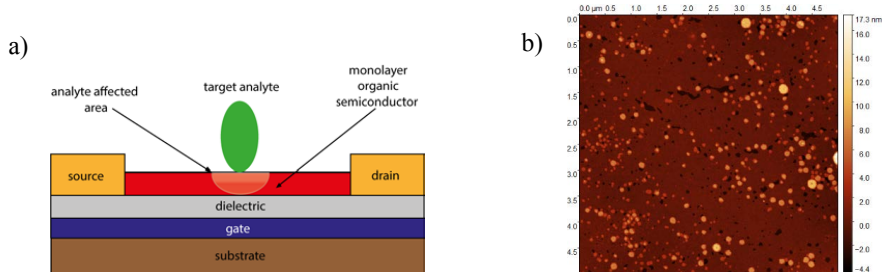


Fig. 1. The illustration of the working principle of the SAMFET-based chemical sensor (a) and the AFM morphology of the Langmuir-Schaefer monolayer (b).

In our work, we investigate sorption and desorption processes of ammonia, hydrogen sulphide and water vapour in Langmuir-Schaefer monolayers of disiloxane derivatives of benzothienobenzothiophene.³ Such films were used as a semiconductor layer of the SAMFETs. The electrical properties of these devices (such as hole mobility, on-off ratio and threshold voltage) were found to be dependent on the concentration of toxic gases and water vapour, allowing such films to be used as a basis for gas sensors. The observed dependence of OFET key parameters is addressed to the reversible sorption of the analyte molecules onto the surface of semiconductor monolayer. Importantly, the analyte sorption occurs only under the gate bias applied, while the unbiased device demonstrates a constant electrical response. These findings indicate a huge potential of Langmuir-Schaeffer semiconducting monolayers for chemical sensing.

This work was supported by RFBR (grant 17-03-00222).

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Novel reactive nanostructured organosilicon luminophores and scintillators on their basis

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The development of efficient, cheap, easy to handle and resistant detectors for both fast and thermal neutrons is of paramount importance in many fields, ranging from nuclear physics to materials analysis and from medicine to new generation nuclear reactors. Usually as the matrix for plastic scintillators used polystyrene (PS) or its derivatives which have a low radiation resistance and a softening point of about 90 °C. Research carried out several years ago has shown that polysiloxanes with aromatic side groups exhibit high radiation hardness and high thermal stability within a wide range of temperatures¹. All of these properties make these materials a good alternative to conventional scintillators in harsh environments.

Earlier, we have reported about nanostructured organosilicon luminophores (NOL)², which have a number of unique properties. In these molecules two distinct chromophores are rigidly connected to each other via a silicon atom, that lead to an intramolecular directional energy transfer from their external chromophores to the center (the so called “molecular antenna effect”³). 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. Selection of chromophores of different structures allows synthesizing compounds with desired optical properties such as absorption and luminescence.

In this work it was suggested to create luminescent organosilicon composites in which NOL are covalently bonded to the organosilicon matrix via terminal reactive groups. For this aim, we have synthesized a number of NOLs which have reactive undecenyl groups on the peripheries⁴. They are responsible for the chemical interaction with the siloxane polymer. As the central luminescence phosphor were used benzothiadiazole and anthracene derivatives with quantum yield up to 95%. The resulting NOLs exhibit emitting wavelengths at 410 - 430 nm (blue), 470-600 nm (green), 570 - 590 nm (yellow) or 640 – 670 nm (red).

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. Their optical properties were studied by fluorescent UV spectroscopy. The scintillation light output and decay time were measured with a single photoelectron counting technique.

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

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Novel donor-acceptor oligomers having different architecture based on triphenylamine 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 electronics¹. Recently a number of star-shaped molecules based on TPA and containing oligothiophene as π -bridges and alkyldicyanovinyl groups as acceptor units have been synthesized^{2, 3, 4, 5}. 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. This work shows the synthesis of a series of oligomers having novel electron donating tris(2-methoxyphenyl)amine core⁶ and novel acceptor units – 3-ethylrhodanine groups⁷. Besides we demonstrate series of push-pull oligomers based on electron-donating TPA and electron-withdrawing dicyanovinyl group.

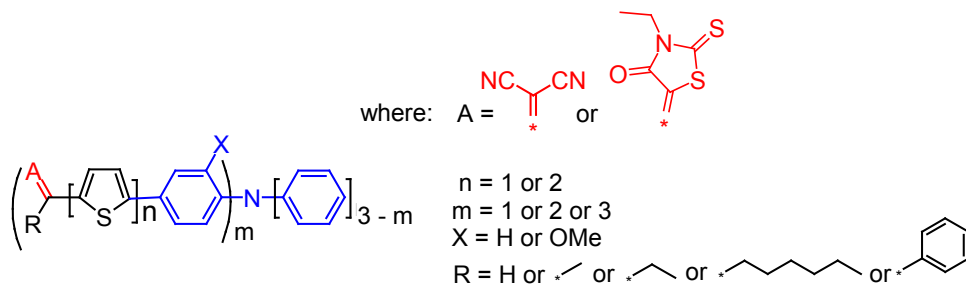


Fig. 1. Schematic representation of star-shaped oligomers based on triphenylamine.

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

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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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Unravelling the mechanism of outstanding electron mobility in F₂-TCNQ single crystals

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High charge mobility is a prerequisite for efficient operation and commercial viability of organic electronic devices, but only several organic semiconductors (OSCs) have demonstrated reproducible charge mobilities above 1 cm²/(V·s), and a few of them have shown band-like charge transport. Search for new high-mobility OSCs requires deep understanding of the charge transport in these materials, and comparative studies of the structurally close OSCs are extremely useful for this purpose. Recently, high band-like electron mobility of about 7 cm²/(V·s) was reported for crystalline 2,5-difluoro-7,7,8,8-tetracyanoquinodimethane (F₂-TCNQ), while mobilities in the crystals of structurally close molecules, TCNQ and F₄-TCNQ, are two orders of magnitude lower¹. Although it was suggested that efficient transport in F₂-TCNQ stems from unusual face-to-face packing¹, the mechanism underlying the impact of the packing motif on the mobility in this crystal family remains unclear.

It is commonly considered that charge transport in OSCs is controlled by interplay of two factors: charge delocalization characterized by the transfer integrals J_i between the adjacent molecules, and charge localization resulting from electron-phonon interaction usually described by the reorganization energy λ . Recently, it was also shown that intermolecular vibrations can modulate J_i significantly and disrupt charge delocalization limiting charge transport². The crystal packing motif determines J_i ; however, it can also modify intra- and intermolecular vibrations².

In the current study, we investigate charge transport in a series of F_n-TCNQ (n=0, 2, 4) crystals by means of combined theoretical and experimental approach. The calculated J_i and λ explain low electron mobility value in F₄-TCNQ as compared to the other two crystals; however, these values do not explain drastic difference in electron mobility between TCNQ and F₂-TCNQ crystals. Moreover, the calculated large λ for an isolated F_n-TCNQ molecule (about 250 meV) contradicts the observed efficient charge transport in F₂-TCNQ, indicating significant intermolecular charge delocalization that can decrease λ . Since this delocalization is very sensitive to the intermolecular vibrations², we investigated low-frequency vibrational spectra of the considered crystals using Raman spectroscopy and solid-state density functional theory (DFT). We found that the frequencies of the lowest modes are significantly higher in F₂-TCNQ that can be a sign of tighter fixation of the molecules in this crystal. The Bader analysis of the periodic electronic density³ confirms this hypothesis showing higher energy of the π - π stacking in F₂-TCNQ. The correlation between the vibrations frequencies, intermolecular interaction energies and electron mobility is discussed from the viewpoint of the transient localization model².

This work was supported by RFBR (project № 16-32-60204).

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Ammonia gas sensors based on fluorinated naphthalenediimide semiconductor films

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Gas sensors based on organic field-effect transistors (OFETs) have attracted a considerable attention due to their light weight, mechanical flexibility, high operational stability and record high sensitivity to specific analytes. Such portable sensors might be particularly useful for healthcare applications, air pollution control on industrial plants and residential sector. Detection of ammonia represents an important task since this poisonous gas is commonly used as a raw material for fertilizers, disinfecting agent at poultry farms and is still in use as a cooling agent. Air pollution with ammonia can cause chronic respiratory diseases and inflammations, so one has to install ammonia sensors at the risky areas to fulfill the safety requirements. At the same time, detection of ammonia and volatile amines is commonly used for food quality monitoring, which represents also a big niche for portable ammonia sensors. Finally, these sensors might be useful for medical diagnostics since ammonia is a marker of such disease as a kidney failure.

Here we report the application of n-type organic field-effect transistors (OFETs) as gas sensors for detection of ammonia. A solution-processible fluorinated naphthalenediimide derivative F-NDI has been designed as a promising air-stable semiconductor material, which was extensively characterized by NMR spectroscopy and X-ray single crystal diffraction. Top-contact bottom-gate OFETs based on F-NDI have delivered a decent mobility ($10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) in combination with a long-term operation stability under ambient conditions. The fabricated devices have demonstrated a good sensitivity and fast response with respect to ammonia, which points towards their high potential as chemical sensors. Some data on the selectivity of the fabricated devices and plausible mechanism of the ammonia detection will also be presented.

This work was supported by Russian Science Foundation (project No. 16-13-10467).

BODIPY as a versatile material for memory elements and photodetectors

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Boron-dipyrrromethenes (BODIPYs) represent an important family of fluorescent dyes, which find applications in lasing, chemical sensors, fluorescent tags for biomedical applications, organic solar cells, light rechargeable batteries and etc. Here we explore the potential of BODIPY dyes as light-sensitive materials for photoswitchable organic field-effect transistors (OFETs), memory elements and photodetectors.

We have shown that introducing a layer of BODIPY dye (Fig. 1a) molecules at the semiconductor/dielectric interface in the OFET structure (Fig 1b) enables light-induced switching of the device. Simultaneous application of light (diode laser $\lambda = 405$ nm) and electric field allows for fully-reversible switching of the device between multiple quasi-stable states, which are characterized by considerably different threshold voltages V_{TH} . The fabricated optical memory elements revealed the switching coefficients between two arbitrary selected states ($K_{SW}=I_{DS(1)}/I_{DS(2)} > 1000$), short switching times (2-10 ms) and decent retention and write-read-erase cycling stability (Fig. 1c).

We have revealed a strong photoinduced conductivity at the BODIPY/ C_{60} junctions, which allowed us to apply them in a planar junction two-terminal devices, operating as highly sensitive photodetectors under forward bias. Fig. 1d shows the response of the photodetector to a series of light pulses with the characteristic time of 0.5 ms, which is limited by the device channel length (100 μ m).

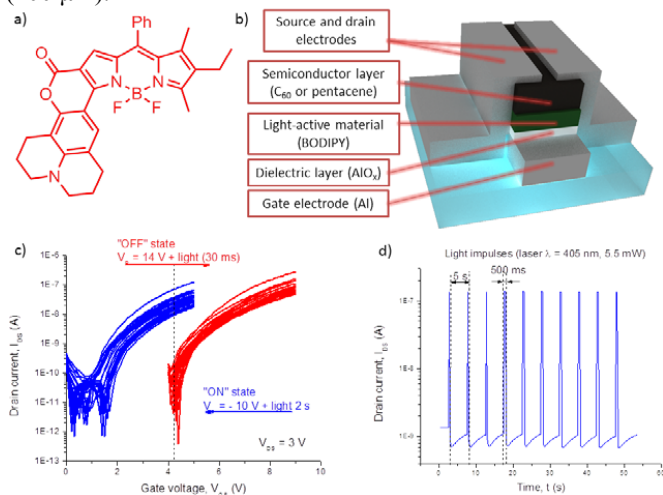


Fig. 1. Molecular structure of the investigated BODIPY (a), schematic layout of the OFET-based memory element (b), switching of the memory device between two distinct states (c), photodetector response to a series of light pulses.

In conclusion, we have shown that rationally designed BODIPY dyes represent promising light-sensitive materials allowing for designing optical memory elements and photodetectors with state-of-the-art characteristics.

This work was supported by RFBR (project № 15-03-06175).

Unsymmetrical donor-acceptor oligomers based on triphenylamine: synthesis and properties

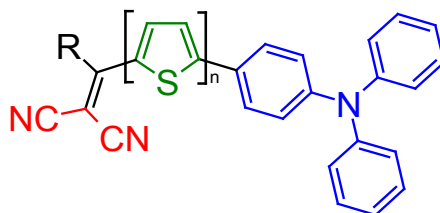
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Donor-acceptor oligomers based on electron-donating triphenylamine and electron-withdrawing dicyanovinyl groups are actively researched as promising semiconductor materials for organic photovoltaics^{1,2,3,4,5,6}. In this work novel unsymmetrical donor-acceptor oligomers based on the triphenylamine with oligothiophene arm end-capped with dicyanovinyl substituent were synthesized, investigated and compared to each other (Figure 1).



where $n = 0, 1, 2, 3, 4$

Fig. 1. Schematic representation of unsymmetrical oligomers

Synthesis of the unsymmetrical donor-acceptor oligomers based on a recently developed synthetic approach using the Knövenagel condensation of the ketone precursors with malononitrile under a microwave irradiation⁷. It should also be noted that their synthesis is more convenient. The unsymmetrical molecules have a low molecular weight that makes it possible to use vacuum sublimation technique for fabrication of organic electronics devices. The electrochemical, thermal and optical properties of molecules were investigated by cyclic voltammetry, differential scanning calorimetry, thermogravimetric analysis and UV-Vis spectroscopy.

This work was supported by The Program of The President of The Russian Federation (grants MK-933.2017.3).

¹ Luponosov Y.N., Solodukhin A.N., Ponomarenko S.A. *Polymer Science, Ser. C* 2014, **56**(1), 105–135.

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³ Ponomarenko S.A., Luponosov Y.N., Min J. et al. *Faraday Discuss.* 2014, **174**, 313-339.

⁴ Kozlov O.V., Luponosov Y.N., Ponomarenko S.A. et al. *Adv. Energy Mater.* 2015, **5**(7), 1401657.

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Effect of space charge limited current under the source and drain contacts on the performance of organic field-effect transistors

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Organic field-effect transistors (OFET) are key basic elements for low-cost, light-weight and large-area electronics. The most important parameter that characterizes the OFET performance is the charge carrier mobility. The common method of mobility measurement in OFET consists in approximation of the OFET transfer characteristics by the Shockley equations in the linear and saturation regimes. However, this method can lead to incorrect estimation of charge mobility in organic semiconductor. In the common staggered device architecture, e.g. top-contacts and bottom-gate OFET geometry, the current needs to pass through the thickness of organic semiconductor layer under the source and drain contacts, and the voltage can drop across the layer due to space charge limited current (SCLC). This can significantly decrease the source-drain current¹ and consequently the apparent (effective) OFET mobility μ_{eff} .

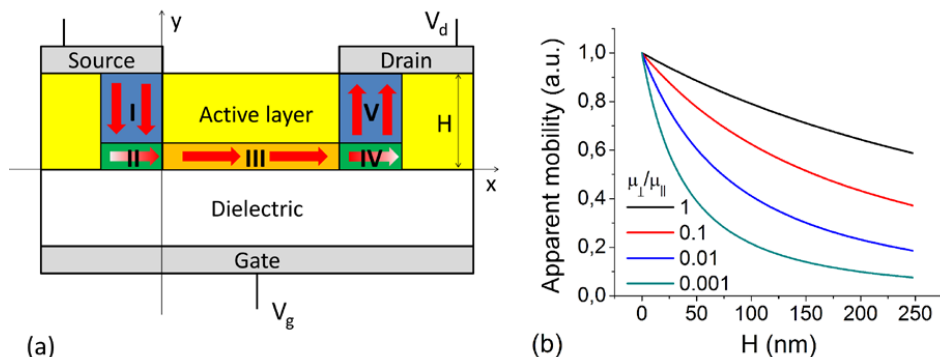


Fig. 1. (a) OFET scheme with areas of current flow. (b) Apparent mobility in the saturation regime vs the active layer thickness H for different mobility ratios $\mu_{\perp}/\mu_{\parallel}$.

In this work, we study how the SCLC under the source and drain electrodes affects the apparent mobility determined from the OFET transfer characteristics. We developed both numerical and analytical OFET models with SCLC under the contacts and found how the fitted OFET mobility changes with the active layer thickness. In the models, the current flow is divided into five areas (Fig. 1a): areas I and V with vertical SCLC, areas II and IV with horizontal increasing/decreasing current and OFET channel III. The modeling showed that the apparent OFET mobility drops with increasing the active layer thickness H and decreasing the intrinsic transverse charge mobility μ_{\perp} (across the active layer) relatively to intrinsic “longitudinal” mobility μ_{\parallel} (along the channel length). These findings allow more accurate evaluation of the intrinsic OFET mobility and provide guidelines for further improvement of OFET performance.

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

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Numerical modeling of power conversion efficiency in organic light-emitting transistors

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Organic light-emitting transistors (OLETs) are novel type of devices which combine light-emitting properties of organic LEDs and electrical switching ability of organic field-effect transistors¹. OLETs contain an organic semiconductor active layer and a dielectric layer and have three electrodes: source, drain and gate (Fig 1a,b). Source injects holes and drain injects electrons into active layer, where electrons and holes recombine, as a result the photons are emitted. By changing the gate voltage the drain-source current can be tuned, therefore the emitted light intensity can also be changed. The OLET efficiency of power conversion from electricity to light is higher than for organic LEDs² but is still lower if compared with inorganic LEDs, partly because of lack understanding of OLET device physics, especially the main energy loss channels. Existing theoretical studies on OLETs do not consider its power conversion efficiency (PCE). This work is devoted to calculation of OLET PCE and quantum efficiency by means of numerical modeling.

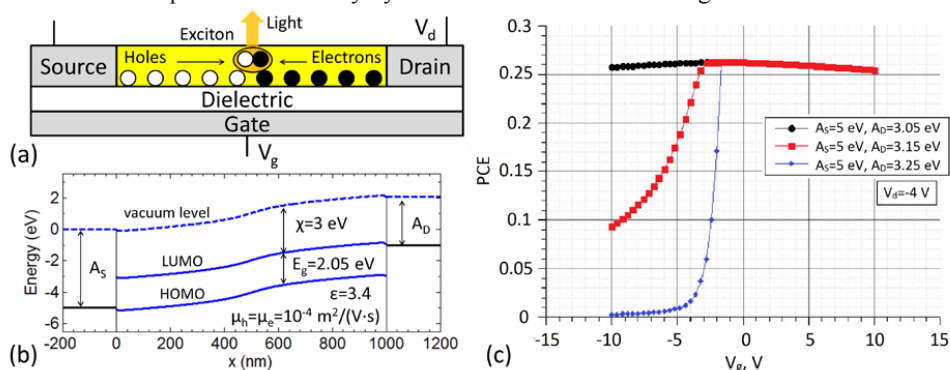


Fig. 1. (a) Scheme of OLET, active layer is shown by yellow rectangle. (b) Band diagram of OLET channel. The values of electron affinity χ , band gap E_g , dielectric permittivity ϵ , hole and electron mobilities $\mu_{h,e}$ are given. (c) Dependences of OLET PCE on source-gate voltage V_g at source-drain voltage $V_d = -4$ V for different source and drain work functions A_s and A_d .

In this work, we present a one-dimensional drift-diffusion numerical model of OLET and study the OLET performance for various parameters and properties of active layer and electrode materials. We have found that the OLET PCE is the most sensitive to the work functions of source and drain electrodes (Fig. 1c). In the same time, the most of geometrical and material parameters of the OLET (such as temperature, electron and hole mobilities, C_s , channel length) give a far less pronounced effect on the OLET performance. We analyze the energy losses due to low carrier mobility, insufficient selectivity and high contact resistance of the electrodes, energetic disorder, and non-radiative recombination. Approaches for minimizing these losses are discussed. The results of this work can help to develop high-performance OLETs.

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

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Influence of a chemical structure of organosilicon BTBT derivatives on their electrical performance in ultrathin OFETs prepared by different techniques

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The aim of the work was to fabricate low-defect ultrathin (close to monolayer) films from novel organic semiconductors by spin-coating (SC), Langmuir-Blodgett (LB) and Langmuir-Schaefer (LS) techniques and compare their morphology, structure and electrical performance of organic field-effect transistors (OFETs) based on them. For this purpose tetramethyldisiloxane dimers (**D2**) of non-symmetrical dialkyl benzothieno[3,2-b][1]benzothiophene (**BTBT**) derivatives with undecyl (**Und**), heptyl (**Hept**) and hexyl (**Hex**) spacers and hexyl end groups – **D2-Und-BTBT-Hex**, **D2-Hept-BTBT-Hex** and **D2-Hex-BTBT-Hex** were synthesized. This choice was based on several reasons: (i) impressive electrical performance of dialkyl derivatives of the semiconductor core – **BTBT**¹; (ii) high air-stability of the semiconductor core² and (iii) possibility to process these dimers by LB or LS self-assembling technique due to disiloxane fragment included into their molecular structure³.

It was found that ultrathin films prepared from all investigated compounds demonstrate the electrical behavior typical for p-type organic semiconductors (Fig. 1).

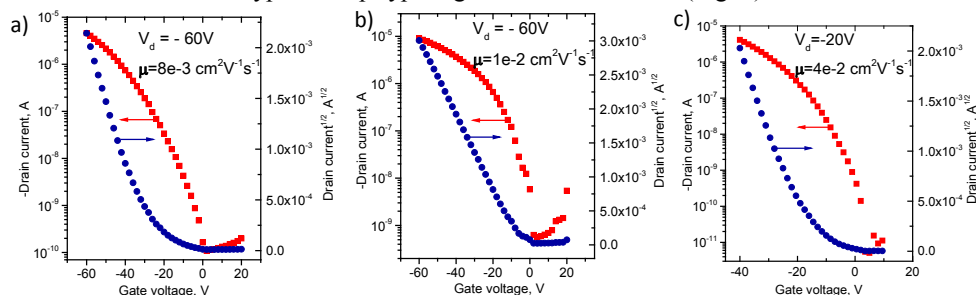


Fig.1 Transfer characteristics of a) **D2-Hex-BTBT-Hex**, b) **D2-Hept-BTBT-Hex** and c) **D2-Und-BTBT-Hex** ultrathin OFETs fabricated by SC technique at optimal conditions.

The average linear mobilities were found to be in the range of $10^{-4} - 10^{-2} \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$. It was observed that alkyl spacer length has a strong influence on the OFETs electrical performance. In the case of SC processing the average linear mobility does not vary significantly with increasing the spacer length from 7 to 11 carbon atoms, but increases in 4-5 times with increasing the spacer length from 6 to 7-11 carbon atoms. In the case of LB and LS processing the average linear mobility has a maximum value for the dimer with heptyl spacer and significantly decreases for the dimer with undecyl and hexyl spacer – in 10 and 20 times, respectively. The electrical performance of prepared devices were found to be very stable at least after three months storage under ambient conditions that enables using them without any encapsulation.

This work was supported by RFBR (projects № 16-29-05321 and 17-03-00222).

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Novel Anthrathiophene-Based Small Molecules as Donor Material for Organic Photovoltaics: Synthesis and Light-Induced EPR Study

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A novel anthrathiophene-based compound, 1,4-bis((5-(6,11-dioxoanthra[2,1-b]thiophene-2-yl)thien-2-yl)ethynyl)-2,5-bis(octyloxy)benzene (Fig.1), was synthesized and characterized¹.

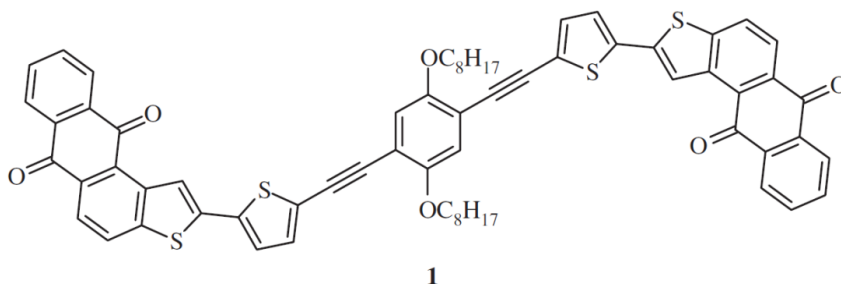


Fig. 1. The anthrathiophene-based compound **1**.

The energies of frontier orbitals were measured by cyclic voltammetry, HOMO = -5.36 eV and LUMO = -3.60 eV. These values show that the compound **1** can act as electron donor in a composite with the widely used fullerene derivative PCBM and as electron acceptor with the widely used semiconducting polymer P3HT. The light-induced radicals **1**⁺/PCBM⁻ and P3HT⁺/**1**⁻ in the composites were revealed by continuous wave and pulse EPR spectroscopic techniques. CW EPR spectra of **1**⁺ and **1**⁻ radicals were simulated by Gaussian lines with 4.2 G and 8G, correspondingly. The optical absorption spectrum and luminescence spectrum of the synthesized compound **1** in film are strongly red-shifted as compared to the same spectra in solution.

The spectroscopic data suggest that the anthrathiophene-based compound is a promising platform for synthesis of both small-molecular electron donors and non-fullerene electron acceptors for organic solar cells.

This work was supported by RFBR (projects № 17-03-01110, № 17-43-543220, № 15-03-07682).

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Influence of the crystallinity of the organic thin film layer in OTFTs

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Charge transport in organic devices depends strongly on the molecular order and morphology of the organic semiconductor thin film. Slight variations on the semiconductor core could play a key role in the molecular packing and charge transport characteristics of organic devices¹. Recently, *N*-trimethyltriindole (**TMT**) has been reported as an organic p-type semiconductor for OTFTs². With this in mind, π -electron enriched derivative 3,8,13-tri(thien-2-yl)-5,10,15-trihexyl-10,15-dihydro-5*H*-diindolo[3,2-*a*:3',2'-*c*]carbazole (**3-TTMT**) has been studied. Surprisingly, the thin film transistors fabricated from **3-TTMT** exhibit lower charge carrier mobility than those fabricated from the parent compound *N*-trimethyltriindole, yielding values of 10⁻⁵ cm²s⁻¹ instead of 10⁻² cm²s⁻¹. The exploration of the relationship between the OTFTs performance and the role of the molecular order in the thin film by grazing incidence X-ray diffraction (GIXRD) is here discussed.

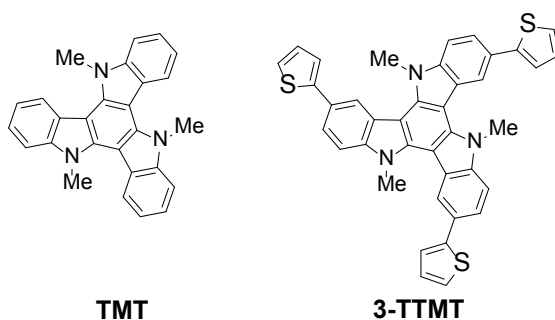


Fig. 1. Organic Semiconductors

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¹ Fengjiao Zhang, Yunbin Hu, Torben Schuettfort, Chong-an Di, Xike Gao, Christopher R. McNeill, Lars Thomsen, Stefan C. B. Mannsfeld, Wei Yuan, Henning Sirringhaus, and Daoben Zhu. *J. Am. Chem. Soc.* 2013, **135**, 2338-2349.

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On the dynamics of additive migration to form cathodic interlayers in OPVs

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A common technique to enhance organic photovoltaic (OPV) performance, is introducing interlayers which either improve charge selectivity or shift the effective work function of the contact. Recently, our group demonstrated the spontaneous generation of cathodic interlayers by migration of an additive to the organic/metal interface during the metal evaporation. This additive/metal interaction reduces the interfacial energy and hence is thermodynamically favored. Therefore, to use this approach for tailoring the organic/metal interface, one should select components that would thermodynamically prefer the active layer: additive phase separation, and apply processing and annealing protocols to ensure this structure. For example, to the OPV working-horse blend, P3HT:PCBM, we added a known cathodic interlayer material: PEG. The affinity of PEG to Al could lead to its segregation to the organic/Al interface during Al deposition. Using XPS and TOF-SIMS measurements we quantified PEG content at the organic/Al interface and found that it is directed by PEG concentration in the blend and/or thermal treatments. Furthermore, the interfacial composition correlated directly with the device parameters. Therefore, by understanding the dynamics of PEG segregation we could quantitatively determine the composition of the buried organic/metal interface and engineer it towards improved performances. These results provide practical insights for judicious selection of additives and processing conditions for interfacial engineering by spontaneous migration of additives.

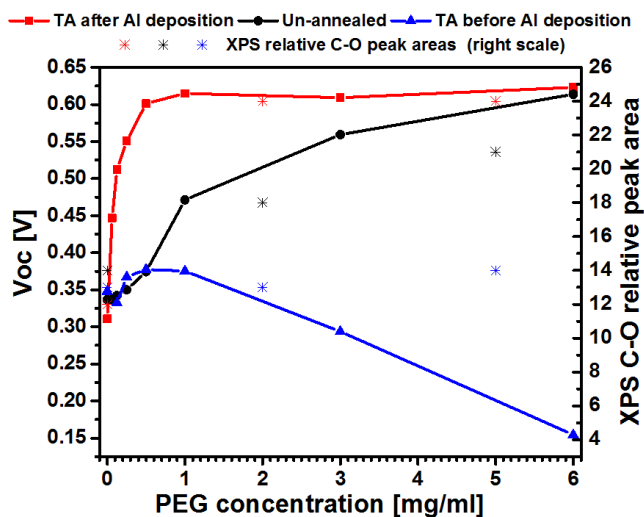


Figure 1- Voc as a function of PEG concentration, for un-annealed devices (black circles), devices annealed prior to Al deposition (blue triangles), and devices annealed after Al deposition (red squares). The stars represent the concentration of PEG at the organic/metal interface as extracted from the XPS measurements of films un-annealed (black stars), annealed prior to Al deposition (blue stars), and annealed after Al deposition (red stars).

Diketopyrrolopyrrole based OTFTs with high performance

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The need for cheap mass production of electronic components and devices is believed to be partially addressed using organic electronics. Among others, mainly material printing is considered as the most promising devices and components fabrication technique. However, in order to overcome certain red brick walls, development of new materials with improved properties is needed. Among the most critical ones in the field of organic thin film transistors fall charge carrier mobility, and material stability and processability.

A common strategy in organic semiconductors development is transformation of old potential suitable pigments into soluble dyes and application them in the construction of new and complex semiconducting materials. The solubilization is usually done via various linear or branched alkyl side chains, e.g. ethylhexyl. While this strategy brings the required solubility and thus better processability, it often leads to increase of molecule distortion, intermolecular distance and reduced charge carrier mobility and thermal stability^{1,2}.

In this contribution, we present study of diketopyrrolopyrrole based organic semiconductors substituted with various solubilization side groups. We show that usage of ethyl-adamantyl³ substituent leads to better molecular packing in solid state through self-organizing due to the bulky adamantane. As a result, this substitution brings high charge carrier mobility of 0.2 cm²/Vs and the material remains soluble. The strategy can be applied for large variety of organic pigments regardless other substitutions by e.g. polar groups. The adamantyl substituents can thus provide useful tool in engineering of molecules for organic and printed electronics.

This work was supported by the Czech Science Foundation via project No. 15-05095S; research infrastructure was supported by Project MŠMT No.LO1211.

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Towards understanding the photochemical degradation pathways of conjugated polymers under anoxic conditions

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Active layer of a bulk heterojunction solar cell generally represents a blend of p-type (conjugated polymer or small molecule) and n-type (fullerene derivative or non-fullerene acceptor) organic semiconductors. These materials undergo photochemical and thermal degradation under the realistic solar cell operation conditions. A thorough understanding of the most important degradation pathways might play a crucial role in improving the long-term stability of organic photovoltaics.

We report a systematic study of three different groups of conjugated polymers (Fig. 1) exposed to continuous UV or white light illumination under anoxic conditions inside the glove box. Gel permeation chromatography (GPC) and fluorescent spectroscopy (FS) have been applied for the first time for monitoring the changes in the molecular weight characteristics of the polymers and reference monomer molecules and accumulation of defects in their thin films.

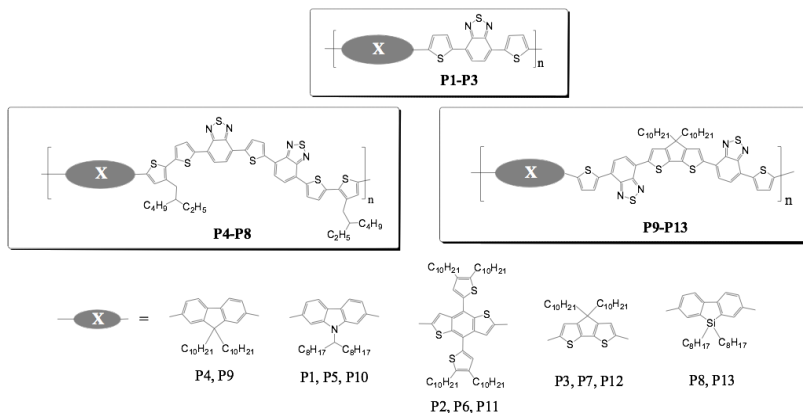


Fig. 1. Molecular structure of investigated conjugated polymers

We have revealed some important correlations between the chemical structures of the certain building blocks incorporated in the polymer chains and their photochemical stability. Light-induced cross-linking of the molecules proceeding presumably *via* [2+2]cycloaddition mechanism has been shown to be the main photochemical aging process. In case of polymers, this kind of cross-linking results in the rapid increase in the molecular weights and, finally, formation of insoluble products.

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Various aspects of organic photovoltaics: the low illuminance and polarization

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Organic photovoltaic cells (OPV) have been expected as low-cost next generation solar cells by printing and coating process. However, for practical use in outdoor applications, serious problems such as improvement of conversion efficiency up to 15% and durability remain. Meanwhile, various applications have already been developed to make use of their unique features such as colorfulness, lightweight, and flexibility. See-through solar cell utilizing its colorfulness is one of excellent application.

In order to make full use of the advantages of OPV, it is necessary to exploit applications based on the only-one features. For example, since OPV shows relatively high performance at low illuminance, it is suitable for energy harvesting under indoor light.

We introduced an LED simulator that can control the illuminance from 1Sun to 200 lx, and which can be tuned to the various spectra of indoor light. Figure 1 shows the low illumination characteristics of the OPV module. As the illuminance decreases, the current sharply decreases, but the voltage decreases little by little. Fill factor (FF) is rather improved, and the reduction of conversion efficiency is relatively suppressed even at the illuminance of 1000 lx, corresponding to 1/100 of 1 Sun.

Besides, molecular orientation controlled OPV utilizing the anisotropy of organic molecules have also been studied, and can be utilized for spin-off technology such as photo-sensors which detect polarized light. The polarized OPV was fabricated by introducing the uniaxial orientation film of p-type polymer semiconductors in heterojunction. The polarization (dichroic) ratio was 2, and a high value of 10 under the monochromatic light. By using the colorfulness of OPV, it is possible to apply it to image sensor which can detect polarized light by RGB.

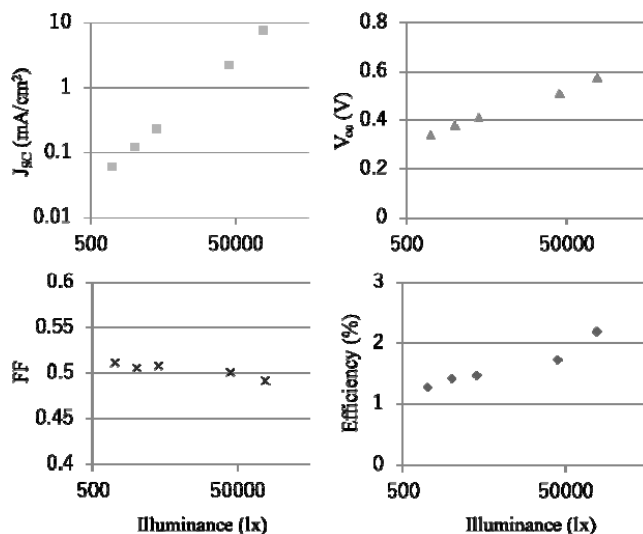


Fig. 1. The dependence of illuminance on PV parameters

High performing solution-coated electrolyte-gated organic field-effect transistors

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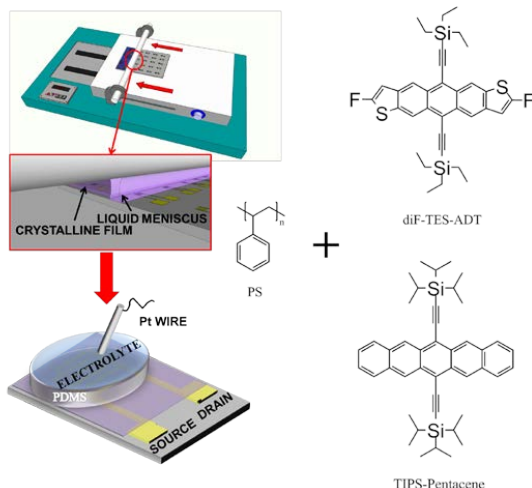


Fig. 1. The BAMS technique and EGOFET along with the chemical structures of TIPS-Pentacene, diF-TES-ADT and PS.

Organic electronics has grown impressively in the last 20 years. To date, the best performing devices are based on single crystal organic semiconductors (OSCs) but, several drawbacks limit their practical use. Regarding polycrystalline semiconductors, different insoluble and soluble OSCs have been successfully employed and processed through ultra-high vacuum sublimation along with spin-coating deposition. However, these deposition techniques still remain quite far from a real industrial upscaling.

We propose a strategy that differs from conventional approaches because it exploits the combination of blended materials together with bar-assisted meniscus shearing (BAMS) technique¹. Our active material is prepared by blending an insulating polymer (e.g. polystyrene) with an organic semiconductor (e.g. TIPS-pentacene, diF-TES-ADT, etc.) yielding thin-films (≈ 30 nm) that display the following advantages: 1) high-crystalline domains, 2) a smooth and compact surface.

The electrical performances were tested by using conventional OFET architecture (*i.e.* bottom gate/bottom contact) and as Electrolyte-Gated Field-Effect Transistors (EGOFETs) where a water droplet acts as gate dielectric. In this configuration a platinum wire, which is the gate electrode, is immersed in the aqueous solution on top of the channel area. The EGOFET is able to work at low operational voltages (<1 V) thanks to the higher capacitance (*i.e.* tens of $\mu\text{F}/\text{cm}^2$) with respect to standard gate dielectrics (*i.e.* tens of nF/cm^2). Our EGOFETs reach excellent performances in terms of mobility as well as subthreshold slope and additionally, show an outstanding stability, which makes them suitable candidates for addressing actual challenges in (bio-)electronics².

This work was supported by ERC StG (project № 2012-306826) and the CSC program.

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Ultrathin, flexible multimodal sensor based on organic field effect transistor for tactile sensing applications.

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To date, one of the most studied field of application of organic semiconductor-based devices is certainly the sensing field. In fact, organic semiconductor-based sensors can be fabricated at low costs on unconventional, highly flexible, and possibly conformable substrates, and can be easily transferred onto clothes for the realization of wearable electronics, or even employed for the fabrication of other interesting applications as flexible smart tags and packaging or even electronic skin. Recently, a rising interest has been directed to the development of novel technologies for reproducing the sense of touch for a large set of possible applications such as prosthetics, human-robot interaction, and rehabilitation.

Low Voltage Charge Modulated OTFTs (OCMFETs) represents a versatile tool for the realization of a wide range of sensing applications and in particular tactile applications. The architecture is based on a floating gate transistor, capable to be operated at low voltages. The sensitivity of the device is obtained by depositing in a part of the floating gate a sensing layer directly exposed to the measurement environment; this sensing layer can be chosen according to the specific external stimulus to be sensed.

In this work we will show that Low Voltage OCMFETs can be fabricated on ultrathin and highly compliant plastic substrates, with a nominal thickness around 1 μm , and employed for the realization of multimodal tactile transducers. In order to achieve sensitivity to temperature, a pyroelectric thin film, namely PVDF, is connected with the sensing area of the device. In this way, when the PVDF temperature changes, the charges induced in the pyroelectric film lead to a variation of the threshold voltage of the OCMFET and, consequently, of the I_{DS} . The proposed approach can be used for temperature monitoring within a range from 8-50 $^{\circ}\text{C}$, which is the typical temperature range requested for tactile applications. Thanks to the piezoelectric property of the PVDF it is also possible to obtain a threshold voltage shift in response to a mechanical stress exerted to the PVDF, thus obtain a modulation of the output current I_{DS} . A detailed dynamic electromechanical characterization has been carried out, showing that such devices are able to detect dynamic stimuli at a frequency up to 500 Hz and we will demonstrate that such devices can detect very small pressure, below 300 Pa and can detect forces within a range from 0.01 up to 5 N.

Interestingly, since the responses of the device to the two different physical stimuli are characterized by marked differences in sensitivity and response time, it is possible to employ the same device for the fabrication of multimodal tactile sensing systems. The highly flexibility of the developed structure, and the easiness of the employed process, make this solution very interesting for the fabrication of multimodal, highly compliant artificial skin.

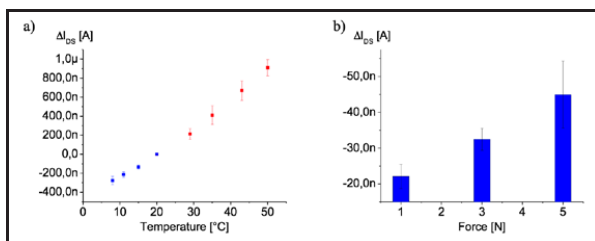


Fig. 1. Current variations VS Temperature (left) and Force (right)

Tuning the Optical Absorption of P3HT Single Crystals for Opto-electronic Applications

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The influence of the crystallization temperatures chosen on the optical properties of self seeded P3HT-26 single crystals has been systematically investigated using the UV-Vis absorption spectroscopy. The degree of planarization of the thiophene rings inferred from the amount of the red shift of the absorption band maximum was found to be better for crystals isothermally grown at high temperatures (T_c) after the successful seeding process. Furthermore, the ratio of the low energy vibronic band to its side band (A_{0-0}/A_{0-1}) and the energy spacing between the A_{0-0} and A_{0-1} vibronic peaks was also found to increase with the crystallization temperature suggesting long-range intrachain interactions along the fully planarized and extended polymer chains. We deduce that highly perfect crystals consisting of polymers with minimum chain folds or extended chains can be grown at reduced growth rates achieved via adopting high crystallization temperatures. It is suggested that high crystallization temperature gives the transportation and attachment processes of molecules to the growth front of the crystal ample time for proper organization leading to good planarization and stacking of chains.

This work was supported by the Deutscher Akademische Austauschdienst, (DAAD), Germany and the National Council of Science and Technology, Kenya.

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Synthesis of new conjugated systems composed of 2,5-di(2-thienyl)pyrrole moieties: investigation of optical and electrochemical properties

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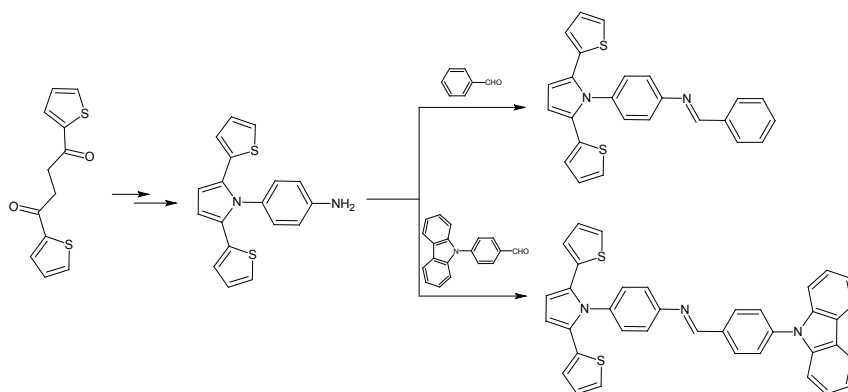
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Synthesis of conjugated polymers, including 2,5-di(2-thienyl)pyrrole (SNS) and carbazole (Cz) moieties has attracted a considerable interest due to the possibility of these compounds to tune the values of their energy characteristics (frontier orbital's energy, bandgap value, triplet energy) and color settings by incorporation of various substituents into their structures. At the same the nature of a linker, which aggregates different units in one molecule, is very essential for the future photovoltaic properties of a created conjugated system. Carbazole-containing compounds are known to have many of useful properties: they easily form stable radical cations, they are good hole conductors with the high carrier mobility, they exhibit thermal and photochemical stability¹. Concurrently the substituted 2,5-di(2-thienyl)pyrroles are known as compounds with good electrochromic properties, low oxidation potentials and good film-forming properties². The Schiff-base linkage is widely used in formation of push-pull chromophore conjugated systems. Here we present the synthesis and investigation of some new conjugated systems, the structure of which includes 2,5-di(2-thienyl)pyrrole and carbazole or phenyl moieties linked through conjugated linkers, which include -N=CH- unit. Electronic absorption and fluorescence spectra were obtained for all the synthesized compounds. Electrochemical properties of new compounds were investigated with the help of the cyclic voltammetry. The surface morphology of the prepared films was studied by atomic force and scanning tunneling microscope NTegro – Prima.



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EGOFETs with immobilized peptide aptamers as biosensors for ultra-sensitive detection of protein biomarkers in complex fluids

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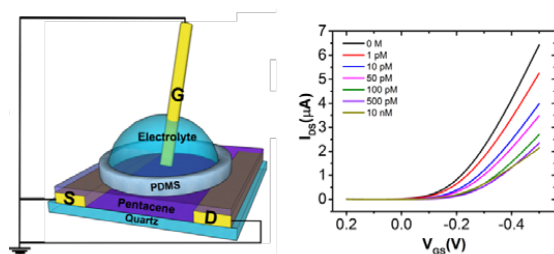
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Optical-based assays have long been indicated as the golden standard of biosensing, thanks to the tremendous sensitivities they ensured, despite the inherent lack of portability due to the need for voluminous equipment and the fact that they often rely on labels. With respect to those techniques, Organic Field Effect Transistors (OFETs) represented a valid alternative. In particular, Electrolyte Gated Organic Field Effect Transistors (EGOFETs) are emerging as key players in the field of biosensing and among the most valid candidates for point-of-care monitoring¹. We have recently demonstrated EGOFET immunosensors for the detection of pro- and anti-inflammatory cytokines², based on immobilization of antibodies with controlled orientation at the gate electrode³. Here, we will present the enhanced sensing performances, in terms of both sensitivity and selectivity, obtained by replacing antibodies with peptide aptamers.



We reached sub-pM limit of TNF α detection (comparable with commercial ELISA kits), even in biological fluids such as cell culture medium containing 10% serum. The functionalization strategy is simple, robust and reproducible, and can be readily translated to virtually any protein analyte of interest. The sensor has been operated in pathology-relevant ranges of TNF α concentrations, demonstrating the potentialities of EGOFET aptasensor in clinical practice.

We gratefully acknowledge IT MIUR Bilateral Project Italy/ Sweden "Poincaré" and "Fondazione di Vignola" for support.

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Structures - electronic properties relationships for the family of five-membered π -conjugated heterocyclic donor-acceptor-donor oligomers

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Recently, we have developed a simple and efficient synthetic route for the preparation of alkyl-substituted esters 2,2'-bithiophene-5-, 2,2':5',2"-terthiophene-5- and 2,2':5',2":5",2"-quaterthiophene-5-carboxylic acids **2**^{1,2}. These esters were converted to conjugated oligomers which contain different electronwithdrawing central units such as 4-phenyl-4H-1,2,4-triazole, 1,3,4-oxadiazole, 1,3,4-thiadiazole, 2,2'-bi-1,3,4-oxadiazole, 2,2'-bi-1,3,4-thiadiazole, 2,2':5',2":5",2"-quater-1,3,4-thiadiazole **3**^{3,4} (Fig. 1).

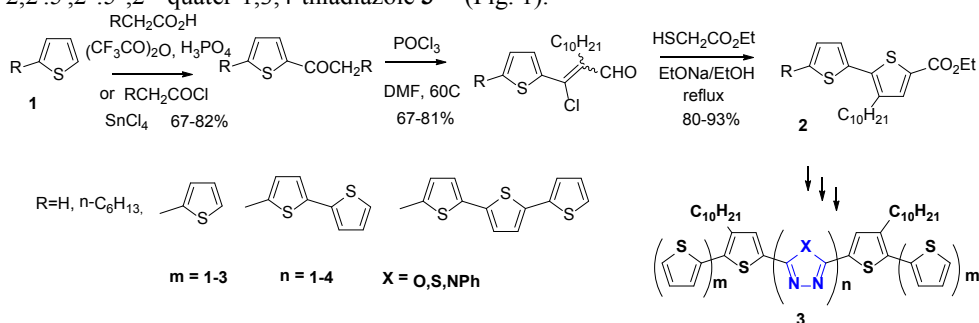


Fig. 1. Synthese of oligomers **3**

The prepared compounds **3** were characterized by electrochemical methods. Ionization potential (IP) and electron affinity (EA) of these molecules were found.

The increase of the conjugation length by incorporation of additional thiophene rings leads to a reduction in the band gap, mostly through increased of HOMO levels. Vice versa, changing the nature of the electron withdrawing heterocycle lead to a greater change the LUMO position.

This regularities allow to predict the frontier orbitals position for the similar compounds and can be used for the synthesis of new semiconductors with the specified properties. These compounds were used as components of active layers in organic light emitting diodes^{4,5}.

This work was supported by the Ministry of Education and Science of the Russian Federation (the project № 4.1657.2017/II4).

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² Kostyuchenko, A.S.; Drozdova, E.A.; Fisyuk, A.S. *Chem. Heterocycl. Compd.* 2017, **53**, 92-96

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⁴ Kostyuchenko A.S., Wiosna-Salyga G., Kurowska A., Zagorska M., Luszczynska B., Grykien R., Glowacki I., Fisyuk A.S., Domagala W., Pron A. *J. Mater. Sci.* 2016, **51**, 2274-2282

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Theoretical Prediction of Operational Stability of Potential OLED Host Molecules by Multireference Quantum Chemistry

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We propose a computational scheme for assessing the operational stability of potential OLED materials. Operational stability of four potential host molecules for blue PHOLEDs is studied based on the bond dissociation energies and exciton energies calculated theoretically using multireference CASSCF/XMCQDPT2 method.

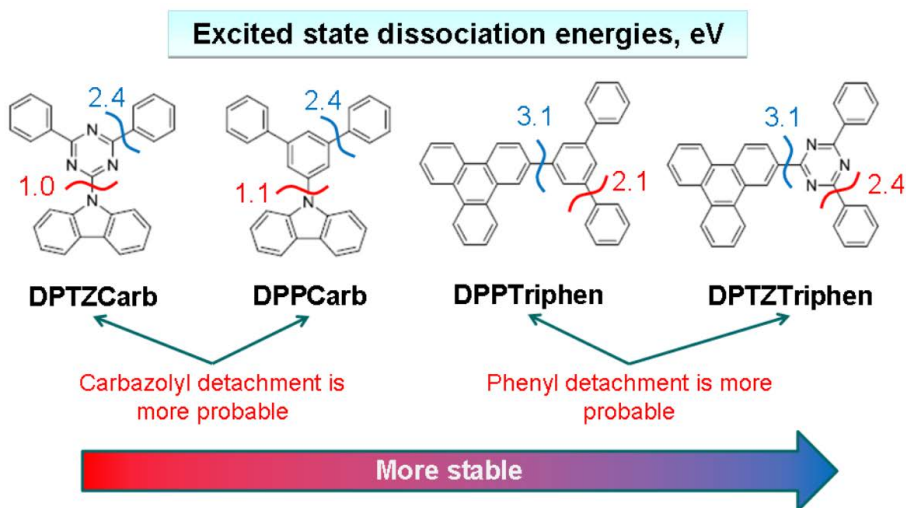


Fig. 1. Studied compounds and stability series with respect to excited-state dissociation

We focused on the degradation through breaking of exocyclic C–C and C–N bonds. The following processes that could lead to the operational degradation of OLED material are considered: the degradation of molecules in charged and excited states and degradation induced by exciton–polaron and exciton–exciton annihilation processes. The dissociation energies are calculated for different exocyclic bonds in the ground, excited, and charged states of these molecules. The least stable states and the most probable dissociation pathways are found. Based on our computations, a stability series is built for the four studied molecules, and the structural features that provide better stability with respect to unimolecular dissociation are determined. Thus, it is found that the carbazolyl group is detached much easier than the triphenylenyl group.

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Introduction of Lambert-function based method for OTFT modelling and application to low temperature measurements

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These last years, printing process has attracted strong interest for the fabrication of organic based sensor directly on flexible surface. Nowadays, organic semiconductors provide performances close to amorphous silicon devices enabling also organic thin film transistors (OTFTs) circuits for the sensors driving and interfacing with conventional electronics.

In this paper, we study a new polymer material (SP400 from Merck) with high mobility (0.5 to 1 cm²/Vs) integrated in P-type OTFTs processed on PEN substrate¹. This materials enables excellent reproducibility, however in-depth characterization and modelling are still to be developed. Here, a Lambert W function extraction method already implemented for inorganic transistors², has been investigated and applied to low temperature (300K down to 125K) measurements for better understanding of the transport in this material.

This fitting model has been validated on transfer characteristics (figure 1a) and their derivative, the transconductance (figure 1b). Then, the low-field mobility (μ_0), threshold voltage (V_{th}) and density of occupied dielectric/semiconductor interface traps (N_{it}) have been extracted. A correlation between the variation of N_{it} and V_{th} with temperature (figure 1c) is observed and will be discussed. Finally, the mobility dependence upon temperature has been analysed with an Arrhenius law model (figure 1d), supporting the hypothesis of thermally activated hopping transport. Furthermore, effective width of localized states and band-like mobility will be extracted³.

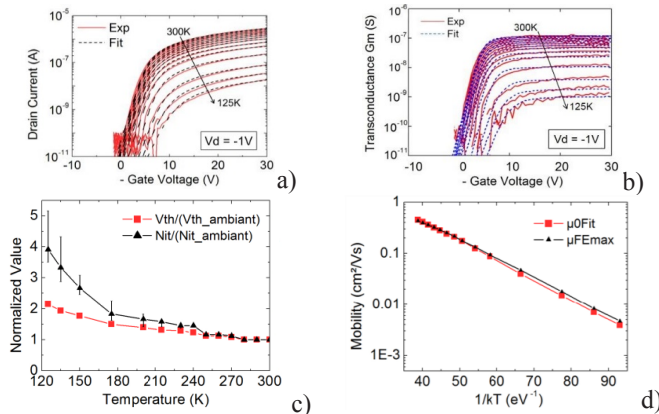


Fig. 1. Experimental (solid lines) and modeled (dashed lines) transfer characteristics (a) and transconductance (b) of a P-OTFT (W/L=2000/20 μ m) with T from 300K to 125K. (c) Evolution vs temperature of V_{th} (red squares) and N_{it} (black triangles) normalized respectively by V_{th} and N_{it} at ambient temperature. (d) Low-field mobility extracted with Lambert function (μ_0Fit) and maximum field effect mobility (μ_{FEmax}) evolution versus $1/kT$ showing an Arrhenius law.

¹ S. Jacob et al., *Proceedings of IEEE International Electron Devices Meeting (IEDM)* 2015.

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³ G. Horowitz, M. Hajlaoui and R. Hajlaoui, *J. Appl. Phys.* 2000, **87**, No 9.

The Nonbonding Conformational Locks for Constructing Highly Planar π -Conjugated Systems

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Nonbonding conformational locks including S...O and Se...O interactions were employed to construct the planar π -conjugated systems. Previously, the alkoxy-functionalized thienyl-vinylene (TVTOEt) building-block with S...O nonbonding conformational locks was employed to construct p- and n-type copolymers for high performance organic thin film transistors (OTFTs) and all-polymer organic photovoltaic (OPV) cells. To further develop the concept, novel building blocks with S...O and Se...O nonbonding conformational locks were designed, synthesized and characterized. The TTVTT(OE) is a novel and highly planar conjugated molecule with S...O nonbonding conformation locks, confirmed by single crystal X-ray diffraction. Interestingly, it is a unique AIE-active molecule that can be used as a biological dye for lipid droplets. Furthermore, the molecule and TTVTT(OE)-based conjugated polymers were employed to construct OTFTs with high charge transport mobilities, which is several orders higher than those of classical AIE molecules. Another novel conjugated molecule SeVSe(OE) has also highly planar conjugated molecule with Se...O nonbonding conformation locks, which was employed to construct p-type and n-type conjugated polymers for high performance OTFTs and OPVs. The Se...O nonbonding conformation locks in SeVSe(OE) were supported by single crystal X-ray diffraction and XAFS. The electron and hole mobilities for SeVSe(OE)-based p- and n-type conjugated polymers are as high as 0.6 and 1.5 cm²/Vs, respectively. The OPV based on SeVSe(OE)-based p-type conjugated polymers are over 6%.

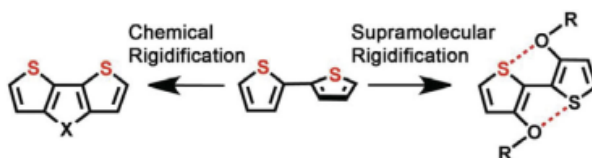


Figure 1. Scheme of Building blocks and Copolymers with Nonbonding Conformational Locks.

Some Complex Bismuth-based Halides as Lead-free Materials for “Perovskite” Solar Cells

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Perovskite photovoltaic materials developed over the past few years demonstrated exciting properties such as high charge carrier mobilities and long diffusion lengths, tunable band gaps, possibility for low temperature film coating from solutions and excellent photon harvesting properties. Extensive efforts on perovskite photovoltaics results in an exponential rise in the power conversion efficiency (PCE), breaking the 20% threshold and coming close to the mainstream silicon PV technology.

Unfortunately, successful commercialization of perovskite photovoltaics is hampered by still poor device operation stabilities in combination with serious concerns regarding to the potential lead poisoning and environmental impact of this emerging technology. This obstacle, however, provides and impetus for intense development of novel lead-free perovskite and perovskite-like absorber materials.

In the present report, we will highlight novel hybrid bismuth complex halides as a feasible replacement for toxic lead perovskites. Synthesis, characterization, thin film processing and photovoltaic performance of novel materials will be discussed.

Substituted Bithiopyranylidenes and their CT Complexes with C60 for Organic Near-Infrared Detectors

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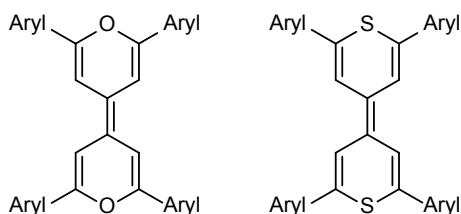


Fig. 1. General molecular structures of aryl-substituted bipyranilidene (left) and bithiopyranilidene (right)

The detection of Near-Infrared (NIR) light has attracted significant interest in the last two decades due to the possible applications in science and industry, such as medical diagnostic, food quality control and communication. An organic photodetector (OPD) has the potential to combine detection of NIR light with the advantages of organic electronic devices such as low-cost, light-weight and high environmental friendliness. The quality of the OPDs depends on an efficient light harvesting process and on a high spectral selectivity in the NIR. However, conventional NIR absorber materials are often missing those prerequisites.

This work investigates the bipyranilidenes and bithiopyranilidenes as classes of materials that exhibit strong charge transfer (CT) absorption in the NIR upon blending with C60. While the charge transfer properties of one bipyranilidene representative were already reported elsewhere¹, this work focuses on identifying and synthesizing the most suitable molecular structure for an application in organic photodetectors. Such a photodetector requires an optical micro-cavity device architecture (concept pioneered at the IAPP) in order to enhance and narrow CT absorption, which is intrinsically weak and broad in nature. Test devices with different bi(thio)pyranilidenes have proven that increasing the electronic density through electron-donating substituents and the exchange of oxygen to sulfur in the pyranilidene core lead to improved characteristics for the tested devices.

¹ Konarev D.V. et al. *Journal of Materials Chemistry* 2000, **10**(4), 803-818.

Molecular FET based on Recombinant Azurin Protein with Enhanced Switching Behavior

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Metalloproteins have been used in molecular bioelectronics as their behavior can be tuned by external potential. Azurin protein from *Pseudomonas aeruginosa* is a copper containing redox protein which transfers electrons from cytochrome c to cytochrome oxidase for respiratory phosphorylation of bacteria¹. Its electron transfer property is exploited for development of transistors², and memory devices³. We have clone the azurin protein in *Escherichia coli* for its overexpression and purification in single step. The protein was characterized by UV-visible, fluorescence spectroscopy and its electrochemical properties were studied by cyclic voltammetry and conductive atomic force microscopy. Also, the recombinant azurin protein is used for the development of field effect transistors based on azurin protein variants where recombinant azurin is used as a channel at 200 nm gap between the gold electrodes.

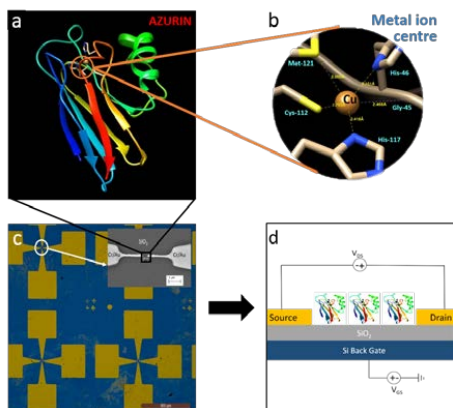


Fig. 1. a) *Pseudomonas aeruginosa* azurin, b) its metal ion center, c) optical image of the device (inset-SEM image), and d) schematic of the device.

Azurin gene from *Pseudomonas aeruginosa* was cloned and overexpressed in large amount. Azurin protein was purified in a single step by Ni-NTA purification. Cyclic voltammograms of recombinant azurin protein immobilized on gold substrate showed clear oxidation and reduction peaks as reported for wild type azurin. The excellent current density of azurin layer on gold was observed in cyclic voltammetry experiments. The Cu containing azurin transistor turns out to be most promising among all with lowest subthreshold swing and high on-off current ratio. The FET device showed consistent behavior in the highly stable mode as measured till 80°C for a span of 8 weeks.

This work was supported by Department of Electronics and Information Technology (DeitY), Government of India

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Influence of electrode materials on highfield polarization and conductivity of the ferroelectric copolymers of vinylidenefluoride and tetrafluoroethylene

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The films of copolymers VDF with TFE composition 94/6 (I) and 71/29 (II) were prepared by crystallization from acetone solution at room temperature. For electric measurements at high voltage device based on the scheme Sayer-Tauer was used¹. Al and Au electrodes were layered by vacuum deposition method. Bipolar high voltage electric field was applied on samples with different frequency and amplitude by using two modes: triangle and rectangle signal. The analysis of time (t) dependences of electric displacement was performed by using a formula²:

$$D = D_i + D_c + D_f = \varepsilon \varepsilon_0 F + \sigma F + 2P_r \left[1 - \exp \left(- \left(\frac{t}{\tau} \right)^n \right) \right] \quad (1),$$

where P_r – remnant polarization, τ - switching time, σ - conductivity of imperfect dielectric. For different sign of electric field which applied by using rectangle mode signal dependences of conductivity σ on the field were estimated. In both sign of field the growth of amplitude leads to increase of conductivity for every type of electrode material. Samples with Au electrodes showed higher conductivity σ in the case of applying negative field than positive one. The difference between conductivities at negative and positive fields for low amplitudes is maximal for the sample of copolymer II. This effect appears both for isotropic and for textured films. It is assumed that these differences are connected with change during the deposition of interface at the metal-polymer surface, which was examined by X-ray photoelectron spectroscopy³. Analysis of Au 4f line shows that on the surface of considering polymers this line is displaced to higher energy compared to pure metal. The comparison of offset value in copolymers with different content of fluorine atom indicates that fluorine causes this effect. Atoms of gold which are deposited on the sample's surface can be involved in formation of double electric layer on the metal-polymer boundary. This process should be accompanied with appearance of hole charges. Consequently, conductivity on the negative semi-period should be higher as such for positive one. An additional argument due to this hypothesis is the fact that inequality of conductivity in different semi-periods of applied field is above in the case of copolymer where fluorine atom content in chain is higher.

This work was supported by RFBR (project № 14-03-00623).

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Synthese of new 5,5'''-bis(3-decyl-[2,2'-bithiophen]-5-yl)-2,2':5',2'':5'',2'''-quater(1,3,4-thiadiazole).

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Bis bithiophene substituted 1,3,4-thiadiazoles and 1,3,4-oxadiazole used as active layers in organic light emitting diodes ^{1,2,3} We have synthesized of new π -conjugated oligomer which contain four serially connected 1,3,4-thiadiazole rings **5** symmetrically substituted by bithiophenes in four steps starting from hydrazide **1**⁴ (Fig. 1).

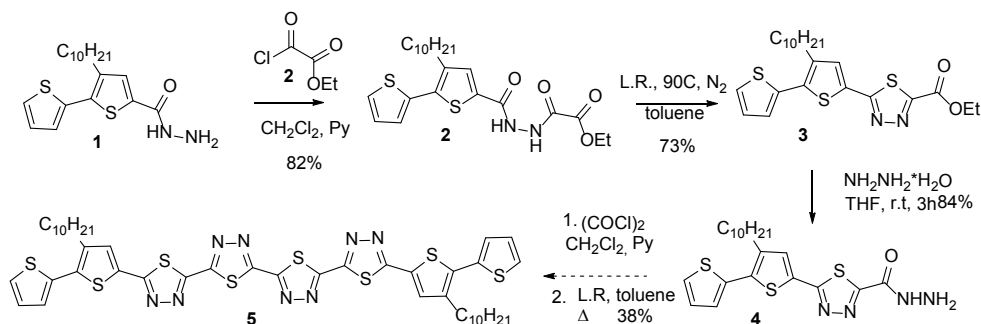


Fig. 1. Synthese of bithiophene quater(1,3,4-thiadiazole) derivative

Electrochemical properties of new octa-ring donor–acceptor π -conjugated oligomer **5** were investigated by cyclic voltammetry. Ionization potential (IP=5.99 eV) and electron affinity (EA=−3.79 eV) of this molecule were found. Two reversibility steps of the charge transfer processes in cathodic potential ranges present on the cyclic voltammogram of compound **5**. The electrochemical bandgap of quater(1,3,4-thiadiazole) is consisted 2.2 eV. Absorption and fluorescence spectra of dilute solutions of quater(1,3,4-thiadiazole) **5** in dichloromethane were recorded. Compound **5** is promising candidate as component of active layer for n-type organic transistors. Compound **5** electropolymerise through terminal thiophene C α –C' α at relatively low oxidation potentials. Electrochemical properties of this polymer were investigated also.

This work was supported by the Ministry of Education and Science of the Russian Federation (the project № 4.1657.2017/IT⁴).

¹ Kostyuchenko A.S., Wiosna-Salyga G., Kurowska A., Zagorska M., Luszczynska B., Grykien R., Glowacki I., Fisyuk A.S., Domagala W., Pron A. *J. Mater. Sci.* 2016, **51**, 2274–2282

² Kotwica K., Kostyuchenko A.S., Data P., Marszalek T., Skorka L., Jaroch T., Kacka S., Zagorska M., Nowakowski R., Monkman A.P., Fisyuk A.S., Pisula W., Pron A. *Chem. Eur. J.* 2016, **22**, 11795–11806

³ Kostyuchenko A.S., Yurpalov V.L., Kurowska A., Domagala W., Pron A., Fisyuk A.S. *Beilstein J. Org. Chem.* 2014, **10**, 1596–1602

⁴ Kotwica K., Kuracha E., Louarn G., Kostyuchenko A.S., Fisyuk A.S., Zagorska M., Pron A. *Electrochimica Acta.* 2013, **111**, 491–498

Improving performance of transistor memory by tuning occurrence charge transport on pentacene interaction

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Nano-floating gate memories have been considered as a promise path to obtain high performance memory devices, because the spatially discrete floating-gate elements effectively act as a charge trapping site. In this work, optimized pentacene thin film transistors have been achieved first by two different self-assembled layers (SAMs) treatments, with surface modification of monolayer octadecylsilane (OTS) on SiO₂ and monolayer pentafluorobenzenethiol (PTFB) on gold source/drain electrodes. Higher mobility and on/off ratio (0.36 cm²V⁻¹s⁻¹ and > 10⁶) are obtained for films deposited on PTFB compared to on OTS. This could be explained by the different occurrence charge transport near the semiconductor/dielectric interfaces and semiconductor/electrodes. According to the analysis of pentacene transistors, different kinds of SAMs treatments of nano-floating gate memories (NFGMs) using gold nanoparticle (AuNPs) charge trapping layer assembled by blocking layer and tunneling layer are demonstrated. The resulting NFGMs with PTFB monolayer exhibited excellent memory performances, including high AuNPs layer charges per unit area, high mobility of 0.053 cm²V⁻¹s⁻¹, the large memory window of 51 V, and reliable cycling endurance over 100 cycles. In particular, the improving performance of the memory devices through tuning the charge transport with SAMs layers suggesting that highlight the utility of surface modulations and controlling of charge transport of interfaces in nanoscale materials.

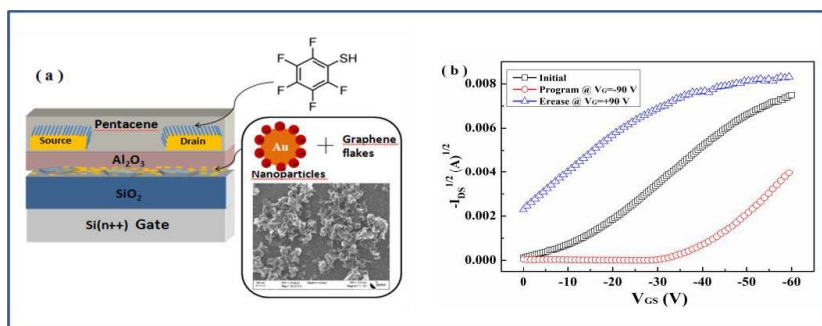


Fig. 1. (a) The architecture and (b) transfer curves of pentacene nano-floating gate memory.

¹ Zhang Jia, Vincent W. Lee, and Ioannis Kyriassis. *Phys. Rev. B* 2010, **82**, 125457.

² S. T. Han, Y. Zhou, and V. A. L. Roy. *Adv. Mater.* 2013, **25**, 5425-5429.

Improving performance of nano-floating memory by tuning occurrence charge transport on pentacene interaction

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Nano-floating gate memories have been considered as a promise path to obtain high performance memory devices, because the spatially discrete floating-gate elements effectively act as a charge trapping site. In this work, optimized pentacene thin film transistors have been achieved first by two different self-assembled layers (SAMs) treatments, with monolayer octadecylsilane (OTS) on SiO₂ and monolayer pentafluorobenzenethiol (PTFB) on gold electrodes. Higher mobility and on/off ratio (0.36 cm²V⁻¹s⁻¹ and > 10⁶) are obtained for films deposited on PTFB. This could be explained by the different occurrence charge transport on pentacene interactions. According to the analysis, the PTFB monolayer treatments of nano-floating gate memories demonstrated excellent memory performances, including high mobility (0.053 cm²V⁻¹s⁻¹), large memory window (51 V), and reliable cycling endurance over 100 cycles. In particular, the improving performance of the memory devices through tuning the charge transport with SAMs layers highlighting the utility of surface modulations and controlling of charge transport of interfaces in nanoscale materials.

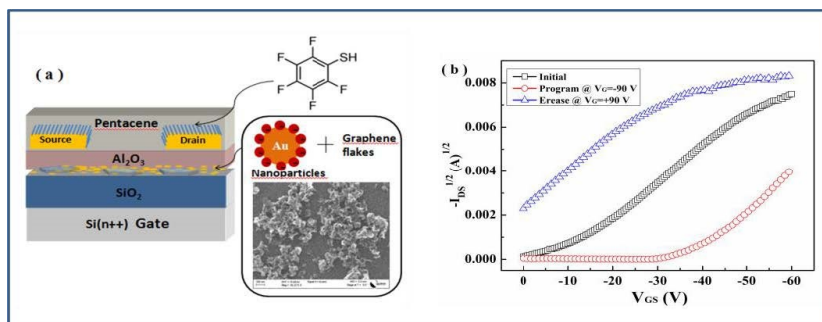


Figure 1 (a) The architecture and (b) transfer curves of pentacene nano-floating gate memory.

Photophysical studies of inclusion complex formation of 3-aminophenol with β -cyclodextrin

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Photophysical studies are carried out on the inclusion behavior of an amine derivative of phenol (3-aminophenol, 3AP) as guest molecule in the host cavity of β -cyclodextrin (β -CD) in aqueous solution. β -CD is very popular as a host for formation of inclusion complex (IC) due to its rigidity and economic availability. Through the encapsulation of a guest molecule in the host molecule, the properties of the guest molecule can be changed, which has a wide utility in drug delivery, sensing, fluorescence on-off system, synthesis of novel material, enhancement of water solubility, etc¹. In the present work, steady state fluorescence emission intensity of 3AP is enhanced gradually with increasing concentration of β -CD, accompanied by a hypsochromic shift as shown in figure 1. Benesi-Hildebrand method² has been used to investigate the stoichiometry of the IC and interestingly found to be 1:1 (Fig. 2). From time-resolved spectroscopic measurements, it is found that the fluorescence lifetime of 3AP increases with increasing concentration of β -CD. All these observations confirm the IC formation of 3AP in β -CD with 1:1 stoichiometry.

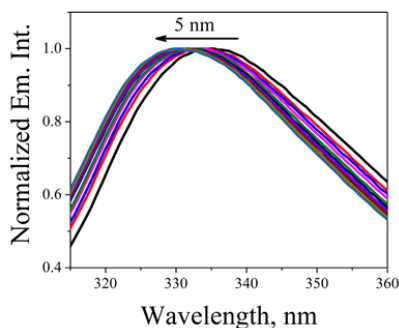


Fig. 1. Normalized steady state fluorescence emission spectra of 3AP in aqueous solution with increasing concentration of β -CD.

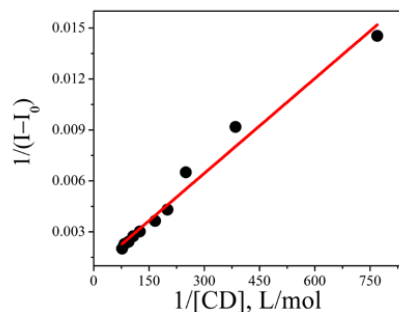


Fig. 2. The B-H plot of $1/(I - I_0)$ vs. the inverse of the concentration of β -CD to determine the stoichiometry of IC in aqueous medium.

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Analytic model of mobility and field-stimulated diffusion coefficient in disordered organic semiconductors

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Charge transport in disordered organics is considered ubiquitously as a hopping process, i.e. it occurs by means of uncorrelated phonon-assisted tunnel jumps of a charge carrier inside a manifold of localized states (LSs). These states are disordered in space and, as a result, in energy, in accord with Gaussian distribution $g(E)$ with mean-square variance σ^1 . Transport level concept is known as an effective analytic tool, which permits to describe hopping transport by relatively simple formalism of multiple trapping (MT) model, which has been developed originally for the case of inorganic disordered materials. The transport level¹ or effective transport energy² is an analog of mobility edge, which separates extended and localized states (traps) in MT model. Up to now, a transport level concept was realized, providing Miller-Abrahams (MA) model of hopping rates between LSs. However, one can show that MT-description of hopping transport does not require application of MA model. Moreover, MT-description does not require introducing the transport energy explicitly. The key assumption is that some small fraction of charge carriers gives the general contribution to charge transport at any time, while others waiting for release from deep states, irrespective to details of hopping mechanism. It is the essence of MT model, and it is typical for disordered organics. Indeed, hopping rates between various pairs of LSs are widely distributed, because of exponentially strong dependence on distance and energy in any reasonable model, since definite fraction of LSs contributes to transport in general (“conductive states”)³. The over assumption is quasi-equilibrium and small occupation of these states (Boltzmann’s statistics), while deep states (traps) can be filled or be far from equilibrium occupation. On the base of these assumptions and the detailed balance principle, one can reduce the well-known balance equation of hopping transport^{1,3} to the balance equation of MT model.

On the base of MT-formalism, differential equation for the spatial- and time-dependent concentration of charge carriers, $p(x,t)$, is obtained. The proposed description of hopping transport is rather universal. Temperature dependence of mobility, as well as temperature and concentration dependence of field-stimulated diffusion coefficient^{1,3}, is analyzed and compared, providing both MA and Marcus hopping rates, in the framework of Gaussian disorder model^{1,4}.

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¹ S. Baranovskii. *Phys. Status Solidi B* 2014, **251**, 487.

² V.R. Nikitenko and M.N. Strikhanov. *Journal of Applied Physics* 2014, **115**, 073704.

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⁴ H. Bässler *Phys. Status Solidi B* 1993, **175**, 15–56.

Development of Polypyrrole-Based Organic Composites in Electrospun Fibers Applied in Bacterial Removal from Surfaces

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The association of bactericidal activity of polypyrrole¹ and available surface area provided by electrospun fibers represents an important condition for development of new biological devices applied in the capture and removal of microorganisms from surfaces. The adequate doping level and oxidizing condition during polymerization represent critical parameters applied in the production of superior organic devices. In this work, we have studied the influence of preparation parameters (such as oxidizing agent and polymerization rate) on morphology, electrical properties and biologic activity of resulting organic fibers. Results reveal that polymerization rate affects the homogeneity of deposition and conjugation length of polymeric chains on electrospun fibers of Eudragit L-100. Figure 1 shows the comparison between pristine (a) and covered (b) fibers by polypyrrole (using ammonium persulfate as oxidant).

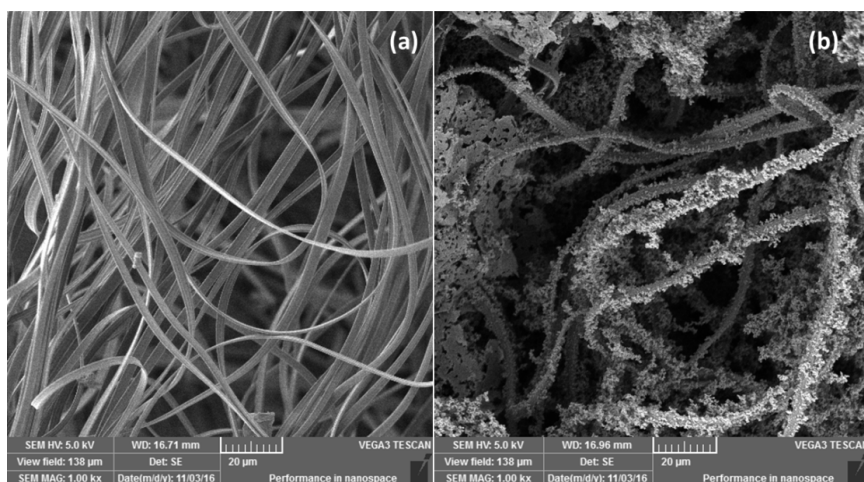


Fig. 1. SEM of pristine fibers of Eudragit L-100 and PPy/Eudragit L-100 fibers.

More homogenous fibers were obtained using ferric chloride, being applied in the adsorption and removal of *Staphylococcus aureus* from surfaces. The resulting nanostructured net returned a strong adsorption of bacteria from surfaces, characterizing a promising candidate for application in organic electronic devices for biology.

This work was supported by CNPq, FACEPE, FAPESB, CAPES and FINEP.

¹ da Silva FAG, Queiroz JC, Macedo ER, Fernandes AWC, Freire NB, da Costa MM, et al. *Materials Science & Engineering C-Materials for Biological Applications*. 2016, **62**, 317-22.

Near-infrared photo detectors based on organic semiconductors

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Organic near-infrared (NIR) photodetectors have tremendous potential in industrial and scientific applications. In this report we report the recent results obtained in our group in this field. Furthermore, the corresponding operation mechanism with different structures and active materials are discussed in detail. Based on NIR absorptive organic small molecules, such as lead phthalocyanine (PbPc), and chloroaluminum phthalocyanine (AlClPc), we fabricated and explored NIR responsive organic photodiodes (OPD)¹ and photo sensitive organic field-effect transistors (PhOFET)²⁻⁶ of various structures. The results showed that the performance of single layer (SL) PhOFETs can be effectively improved by optimization of substrate temperature² as shown in Fig.1 and introducing an inducing layer³. For NIR PhOFETs based on PbPc/C60 planar heterojunction (PHJ), high responsivity of 21 A/W was obtained by replacing SiO₂ with polyvinyl alcohol (PVA) as the gate dielectric⁴. NIR PhOFETs adopting homo type PHJ pentacene/PbPc showed much better air stability than its iso-type counterpart⁵. We proposed a novel structure of hybrid planar-bulk heterojunction for the active layer of PhOFETs, which was demonstrated to be superior than the PHJ and bulk heterojunction⁶.

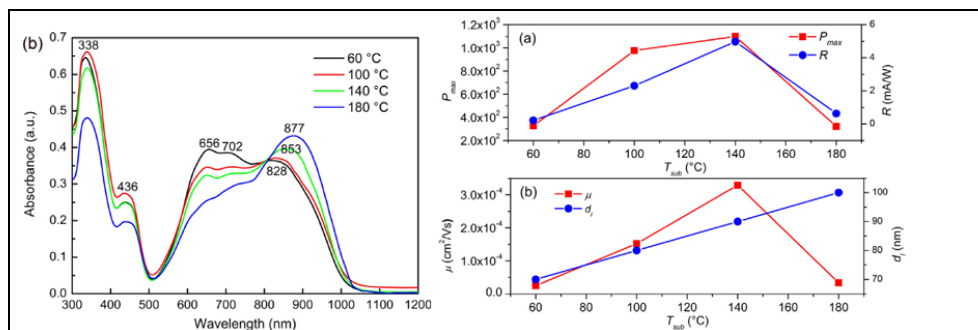


Fig. 1. The Substrate temperature dependence of optical absorption of PbPc thin films and device performances.

This work was supported by National Program on Key Research Project Grant No. 2016YFF0203605.

¹ Lv W., Peng Y., Zhong J., Luo X., Li Y., Zheng T., Tang Y., Du L., Peng L. *IEEE Photonic Tech. L.* 2015, **27**(9), 2043-2046.

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⁶ Peng Y., Lv W., Yao B., Fan G., Chen D., Gao P., Zhou M., Wang Y. *Org. Electron.* 2013, **14**, 1405-1051.

Broadband photodetectors based on organic semiconductor

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Organic broadband photodetectors have tremendous potential in industrial and scientific applications. In this poster we report the recent results obtained in our group in this field. Furthermore, the corresponding operation mechanism with different structures and active materials are discussed in detail. Based on organic small molecules with complementary optical absorption, such as fullerene (C60), 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA), copper phthalocyanine (CuPc), chloroaluminum phthalocyanine (AlClPc), and lead phthalocyanine (PbPc), we fabricated and explored broadband responsive organic photodiodes (OPD)¹ and photo sensitive organic field-effect transistors (PhOFET)²⁻³ of various structures. The results showed that the performance of broadband photodetector can be effectively improved by optimization of component¹ as shown in Fig.1, and changing the gate dielectric³. Hybrid organic-inorganic photodetectors based on three-component bulk heterojunctions achieved ultrahigh photosensitivities of 30-50 A/W at ~0.1 mW incident optical power¹. Broadband PhOFETs adopting hetero type PHJ C60/AlClPc showed high photoresponsivity and fast time response². For broadband PhOFETs based on C60/(PTCDA:AlClPc) hybrid planar-bulk heterojunction (HPBHJ), high responsivity of 2.44 A/W was obtained by replacing SiO₂ with polyvinyl alcohol (PVA) as the gate dielectric³.

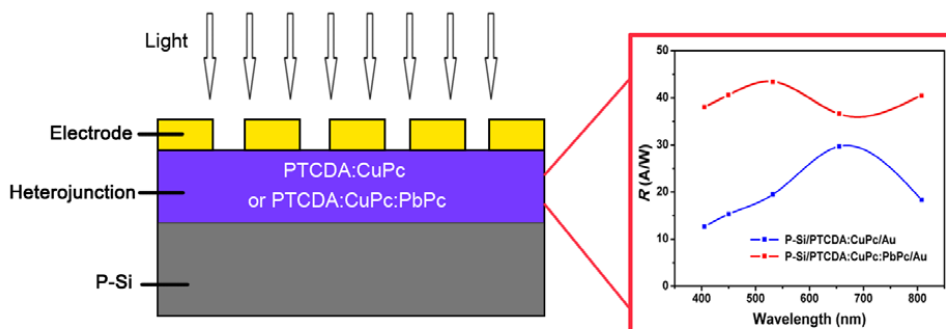


Fig. 1. Schematic 2D view of hybrid organic-inorganic photodetectors based on multiple component organic bulk heterojunctions and the wavelength dependence of photoresponsivity.

This work was supported by National Program on Key Research Project Grant No. 2016YFF0203605.

¹ Zhao F., Luo X., Liu J., Du L., Lv W., Sun L., Li Y., Wang Y., Peng Y. *J. Mater. Chem. C* 2016, **4**(4), 815-822.

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Enhanced efficiency of light upconversion *via* emitter structural modification

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Light upconversion (UC) *via* triplet-triplet annihilation remains extremely interesting topic over the decades because of relatively low power densities ($\sim \text{mW}/\text{cm}^2$) required for the process to take place. The low power UC is considered to be very promising for enhancing performance of photovoltaic cells, since the power density of the sun light is sufficient to accomplish the conversion of otherwise unusable infrared radiation. The efficiency of UC in a solution, due to high molecular diffusion, exceeds 30%, however for the practical usage of UC in photovoltaics, the solid state is more desirable. Yet, the efficiency in the solid state is more than one order of magnitude lower as compared to solution.¹ Although all the factors contributing to the efficiency drop are still unclear, most of them are mainly associated with the self-quenching of an emitter such as 9,10-diphenylanthracene (DPA). Therefore, to retain high UC efficiency, the new emitters with modified molecular structure capable of reducing self-quenching at high concentrations are needed. In this work, the UC properties of structurally modified DPA derivatives were investigated in polymer films. Quantum efficiency measurements of UC performed as a function of emitter concentration revealed that the modified DPA derivatives allow achieving almost twice as high concentration as compared to unmodified DPA without substantial quenching, which results in attaining over 2% maximal UC efficiency in the solid polymer films.

¹ Raisy R., Kazlauskas K., Jursenas S., Simon Y. *ACS Appl. Mater. Interfaces*. 2016, **8**, 15732-15740.

Facile Synthesis, Fluorescence and OFET Properties of Larger Fluorenes

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π -Expanded 2D fluorenes were synthesised via double annulation at 2,3 and 6,7-faces of fluorene employing DDQ-mediated oxidative cyclization method^{1,2} with very high regioselectivity. The larger fluorenes thus obtained were found to be rigid and planar. This led to near-UV absorbance, bright blue emission with very high close-to-unity fluorescence quantum yields, and deep HOMO energy levels with excellent thermal stabilities³. In addition, single crystal X-ray analyses of the newly synthesized fluorenes revealed potential π - π stacking that is found to depend on the substituents at either 9-position or the aromatic ring. We have fabricated solution-processed OFET devices for these electron-rich fluorenes and have characterized their charge transport performances. Some of these interesting results will be presented herein.

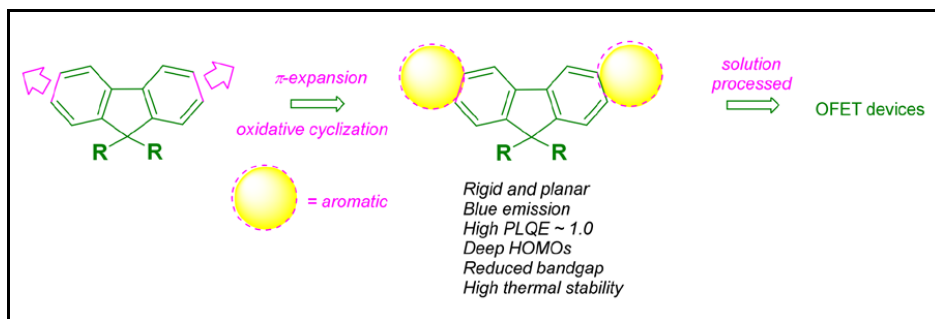


Fig. 1. Synthesis of π -expanded fluorenes and their functional application in OFETs.

This work was supported by DST-SERB (SB/S1/OC/2014) and CSIR (02-0185)/13/EMRII New Delhi, India.

¹ Zhai, L., Shukla, R., Rathore, R. *Org. Lett.* 2009, **11**, 3474.

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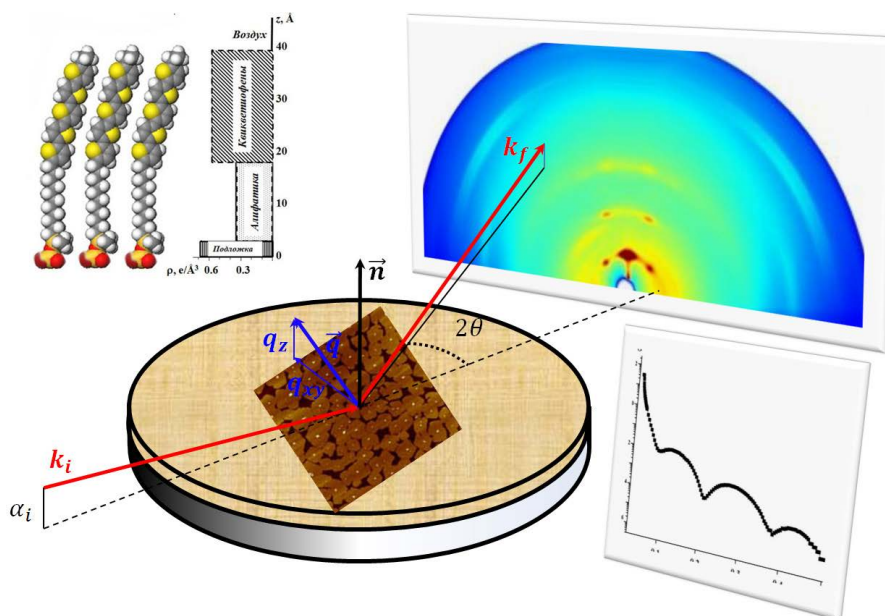
Modern approaches to the studies of thin films: X-Ray reflectometry and grazing incidence scattering

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Modification of the surface of materials by thin-film coating with the aim of conferring them with special properties is an important approach of modern materials science. The properties of such coatings and their operating characteristics are determined primarily by their structure. In this work, modern methods of research of nanoscale thin films of different nature, based on the effect of total reflection and scattering of X-rays from the surface (X-ray reflectometry, grazing incidence diffraction) are presented. A number of examples of the studies of self-assembling macromolecular systems with (semi) conductor properties which are perspective materials for the production of thin-film transistors, light emitting diodes, photovoltaic cells, are shown



This work was supported by RFBR (project № 15-03-05919).

Comparative analysis of the structure and phase behavior of carbosilane dendrimers based on α,α' -dialkylquattrothiophene

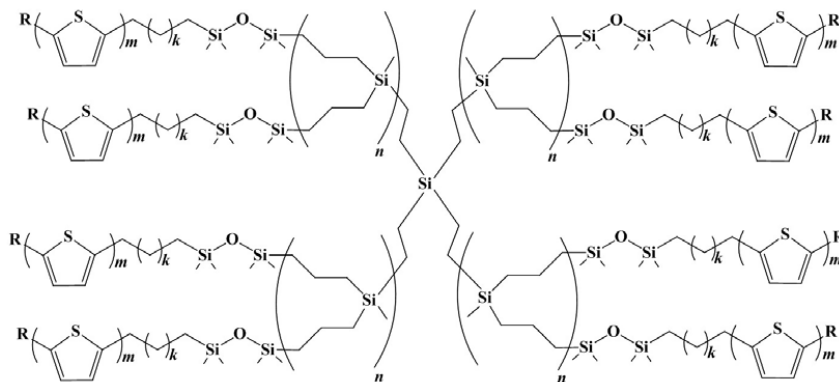
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Organic electronics is a new growing field of materials science, aiming at creating low-cost, flexible, light, large-area devices, the main elements of which are organic thin-film transistors, light-emitting diodes and photovoltaic cells. Such devices are not an alternative to the existing silicon electronics, as they have comparatively low operating frequency due to relatively low charge carrier mobility. At the same time, organic electronics opens new possibilities for its application due to their flexibility and light weight. In addition, relatively low production cost of organic devices could be achieved by replacing expensive processes used in the manufacture of traditional solid-state electronics by cheaper printing technologies. Therefore, in the recent years great importance is attached to the search and design of new conjugated organic structures with high carrier mobility, conductivity, high luminescence efficiency, good solubility and other properties required to create more efficient materials and technologies for organic optoelectronics.

This work is devoted to the development of new approaches for the rational design of self-assembling systems for advanced electronics and optoelectronics. Comprehensive study was conducted for the structure and properties of organosilicon derivatives of α,α' -dialkyloligothiophenes – dendrimers of different generations with a variable number of end groups: $n = 4$ (generation 0), 8 (first generation G1), 19 (third generation G3), 60 or 115 (fifth generation G5).



Formation of smectic layered structures in which amorphous regions of aliphatic tails alternate with herring-bone crystallites of oligothiophene, was observed. Cross-sections of the unit cells of such crystallites by 001 planes are close to that of polythiophene orthorhombic crystal lattice. The period of the alternation is determined by the chemical structure of the molecule - the ratio of the lengths of aliphatic endings kvattrotiufenovyh fragments and aliphatic spacers. Direct correlation between the cross-sectional area S of the unit cell and the electric charge carrier mobility in the samples was revealed – the less the value of S , the better the conductivity of the material. Interaction of oligothiophene fragments leads to the formation of extended areas serving as 3D conducting sheets. Possibility of the formation of extended ordered structures in the studied compounds show the prospects of their application in modern photoelectronics.

Photo-oxidation of Electron Acceptors and their Blends

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The efficiency of solution processed organic solar cells is approaching the threshold for commercial viability^{1,2}. However, before commercialisation, the major challenge of improving stability must be overcome. Stability research mainly focuses on that of the donor polymers, leaving the acceptor much less studied and its impact on overall device stability unclear.

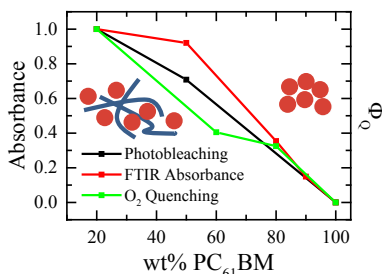


Fig. 1. Fractional loss of UV-Vis absorbance, relative growth of C=O FTIR signal and relative yield of triplet states quenched by oxygen, as a function of wt% PC₆₁BM, following 1950, 970 and 0 minutes of photo-aging, respectively.

Here, the photo-oxidation of the fullerene derivative [6,6]-phenyl-C₆₁-butyric acid methyl ester (PC₆₁BM) was investigated as a neat film and when blended with the photo-inactive polymer polystyrene (PS). The blend films were found to be significantly more susceptible to photobleaching than the neat film, corresponding with the appearance of a carbonyl FTIR absorbance band, and oxidation likely occurring via exoxidation³. This enhanced photo-oxidation correlated with increased oxygen quenching of PC₆₁BM triplet states, suggesting PC₆₁BM photo-oxidation is primarily due to triplet-mediated singlet oxygen generation. PC₆₁BM neat films were observed to undergo sufficient photo-oxidation for even modest (≤ 40 mins) irradiation times, degrading electron mobility substantially, indicative of electron trap formation due to a deepening lowest unoccupied molecular orbital level. These results have important implications on the environmental stability of PC₆₁BM in optoelectronic devices, including in organic solar cells and as the electron transport layer in perovskite solar cells. Alternative non-fullerene acceptor materials were also studied and compared with PC₆₁BM.

This work was supported by the: National Research Network in Advanced Engineering and Materials; Welsh Assembly Government funded Sêr Cymru Solar Project; EU Cheetah project; and Imperial College Junior Research Fellowship scheme

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² Liu, Y., Zhao, J., Li, Z., *et al.* *Nat. Commun.* 2014, **5**, 5293.

³ Xiao, Z., Yao, J., Yang, D., *et al.* *J. Am. Chem. Soc.* 2007, **129**, 16149.

Manifestation of T-exciton Migration in the Kinetics of Singlet Fission in Organic Semiconductors

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Kinetics of singlet fission in organic semiconductors, in which the excited singlet state (S_1) spontaneously splits into a pair of triplet (T) excitons, is known to be strongly influenced by back geminate annihilation of TT-pairs.

We show that this influence can be properly described only by taking into account the diffusive exciton migration. The T-exciton migration effect is treated in the model of two kinetically coupled states: the intermediate [TT]-state (at short distances) of the pair of interacting T-excitons and [T+T]-state of separated T-excitons, undergoing three-dimensional diffusive migration outside the intermediate state. Within this model the kinetics of singlet fission (including magnetic field effects on the kinetics) is studied as applied to the fluorescence decay kinetics (FDK) $I_{S_1}(t)$ for S_1 -state.

The analysis shows that the FDK $I_{S_1}(t)$ decreases exponentially at short times and much slower (as inverse power type function of time) at long times. The T-exciton migration is found to strongly manifest itself in the FDK resulting, in particular, in the universal asymptotic long time dependence $I_{S_1}(t) \sim t^{-3/2}$. The manifestation of the migration, however, appears to be quite distinguishable at intermediate times of evolution in [TT]-state. The model accurately describes the FDK $I_{S_1}(t)$, recently observed at times $10^{-1} \text{ ns} < t < 10^2 \text{ ns}$ for a number of amorphous and crystal systems.

Possible applications of the considered model to the analysis of mechanisms of migration, using experimentally measured FDK, are briefly discussed. In particular, the model is expected to be sensitive to details of the mechanism of T-exciton migration and TT-interaction, and therefore can be suitable for studying specific structural properties of organic substances (solid and liquid) and singlet fission processes in them by analyzing the FDK in a wide region of times $t \leq 10^2 \text{ ns}$

Resonant Energy Transport in Dye-Filled Monolithic Crystals of Zeolite L: Modeling of Inhomogeneity

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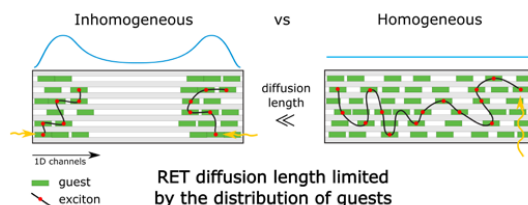
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Resonant energy transfer (RET) is a key mechanism in organic optoelectronic devices, and its efficiency depends critically on the intermolecular arrangement of the active compounds. Supramolecular organization promoted by nanostructured supramolecular host-guest compounds (HGCs) is an elegant way of controlling the packing of the molecules inserted in optically inert organic or inorganic host materials. Under ideal conditions (i.e. dye properties and homogeneous distribution) very high exciton diffusion rates are expected in Zeolite L HGCs, being of high relevance for practical applications. From experiment however, there is clear evidence for inhomogeneity dependent on the type of the chromophores, the preparation procedure, and the size of host crystals, but the reason for inhomogeneity and the consequences on exciton diffusion are under debate. In this work we elucidate these issues making use of computational tools (dynamic Monte Carlo and molecular dynamics) to elucidate the RET dynamics in the inorganic Zeolite L taking into account the inhomogeneity of the dye distribution along the 1D channels.



Satellite Event

Towards Roll-to-Roll upscaled high efficient Perovskite based flexible solar cells and modules

*R. Andriessen*¹

¹Solliance, program director

The interest to Perovskite Solar Cells (PSC) is drastically increased since the last few years. High power conversion efficiencies (certified world record is currently 22,1%), low-cost potential and the flexibility potential make PSC a very promising candidate for future PV applications as there are: (i) rigid (glass-based) single junction panels for low cost PV utility plants, in (ii) in cSi/PSC tandem modules where a semi-transparent PSC can be applied and last but not least (iii) in flexible single junction PSC modules, produced R2R, opaque or semi-transparent that can, as PV product, further integrated on 2D, 2,5D or even 3D surfaces of (public) infrastructure elements, building elements and transport vehicles.

The low cost potential is based on the cheap earth-abundant materials, the very thin electro-active layers and possibility of low temperature and ambient S2S or R2R processing.

To bring Perovskite PV technology to the market researchers and engineers at Solliance and its industrial partners are working on the most challenging topics required for the future S2S and R2R manufacturing, such as: (i) optimization of a generic device stack providing high efficiency and long operational stability; (ii) develop and optimize cheap and non-vacuum processes for the electro-active materials, including R2R slot die coating and R2R spatial ALD; (iii) optimization of the slot die coating process for the perovskite layer; (iv) developing advanced module designs using laser system and (v) developing application oriented packaging technologies. The presentation will update on:

- Efficiency status for single cells for different stack designs;
- Efficiency status of lab scale modules
- Efficiency status of upscaling processes, both S2S and R2R
- Laser interconnections and design of the modules
- Efficiency status of up-scaled modules
- Stability assessment (humidity, temperature, light, electrical bias, combinations) improvements thereof by device, chemical, process engineering
- Status of packaging technologies and approaches
- Further applications for Perovskite based PV

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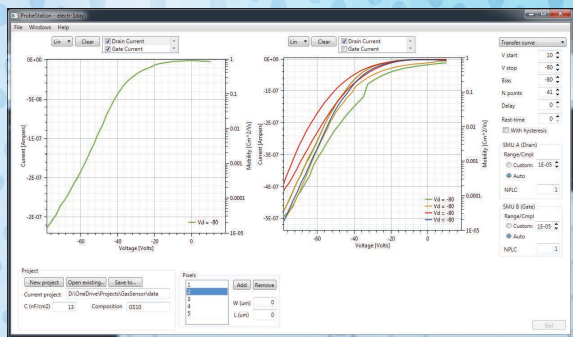
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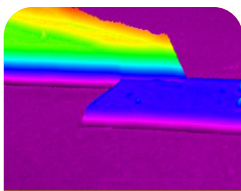
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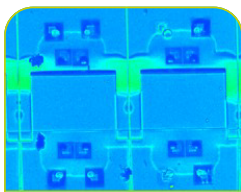
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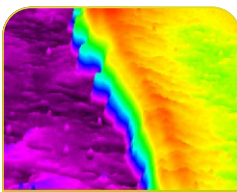
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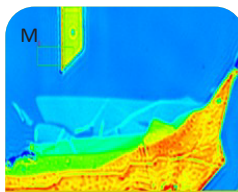
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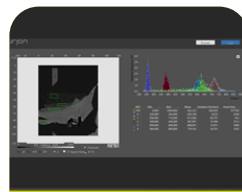
Ellipsometric contrast at 260 nm
MEMS | Si



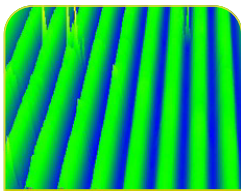
Thickness map
PEDOT | ITO | PET (foil)



Ellipsometric contrast
 MoS_2 (Monolayer) | Sapphire



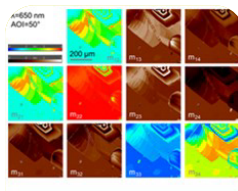
Data Studio: The new way of
doing ellipsometry



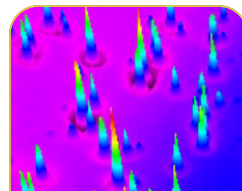
Refractive index map
 As_2S_3 | glass



EP4_Model
Intuitive and easy to use



Müller Matrix Micromaps
Thiophene oligomers

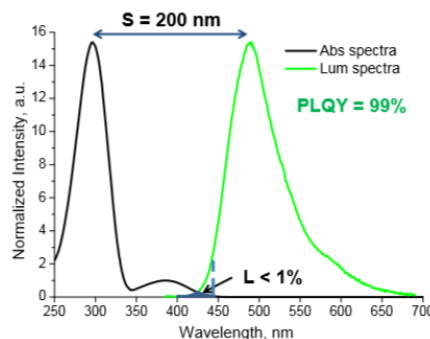


Thickness map
Air|PCBM (spin-coated)|gold

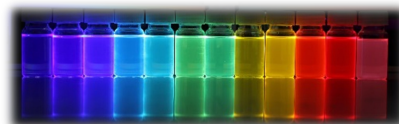
The main goal of LumInnoTech is research, development and commercialization of Nanostructured Organosilicon Luminophores (NOLs) with unique optical properties combining those of organic luminophores and inorganic quantum dots.

Key advantages of NOLs:

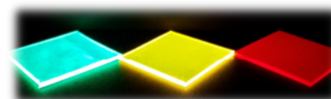
- High luminescence quantum yield: *up to 99%*
- High molar extinction coefficient: *up to 300 000*
- Large pseudo Stokes shift: *up to 250 – 300 nm*
- The possibility of controlling a wavelength of the light emission in a wide range
- Good solution processability
- High stability



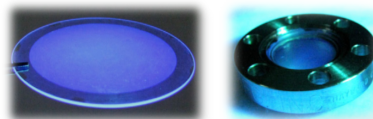
» **A library of NOLs, emitting at the desired wavelengths in the range from 390 to 650 nm.**



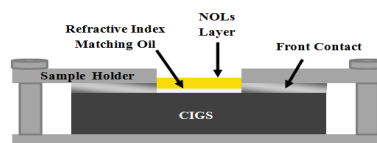
» **Wavelength shifting plates for pure CsI crystals**



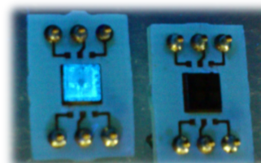
» **VUV wavelength shifters for improving photon detection efficiency of noble gas detectors**



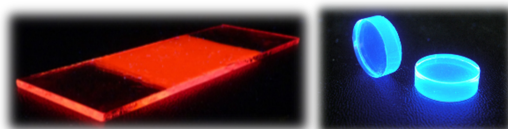
» **Luminescent Down Shifting Materials for CIGS Photovoltaics**



» **Effective Spectral Shifters for Silicon Photomultipliers**



» **New generation of highly efficient and fast plastic and organosilicon scintillators**



» **Various NOLs are available from 100 mg to 100 g quantity**

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