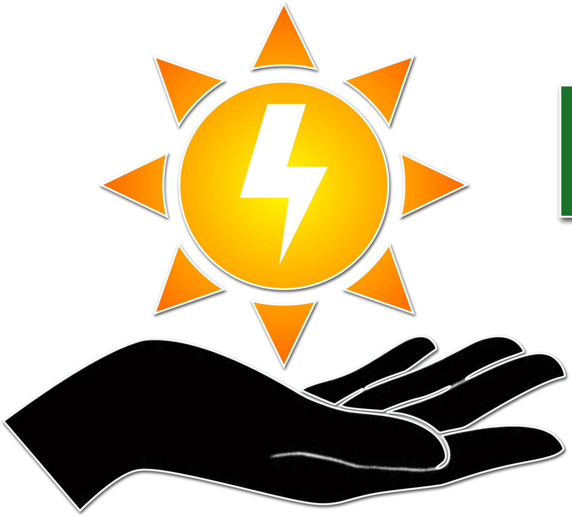

HOPE-PV 2025

The 6th International School on Hybrid, Organic and Perovskite Photovoltaics

BOOK OF ABSTRACTS

FRC PCP MC RAS, Moscow - Chernogolovka, 9 July 2025

Organizer

Federal Research Center for Problems of Chemical Physics and Medicinal Chemistry of Russian Academy of Sciences

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Scientific program

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Invited Lectures

The development of novel electron transport layers to improve the efficiency and stability of perovskite solar cells

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Electron transport layers (ETLs) play a critically important role in enhancing the efficiency and stability of perovskite solar cells (PSCs). Therefore, the development of novel ETLs with tailored properties is a key factor for the commercialization of this technology. This study systematically investigated small-molecule, dimeric (PDI-X-PDI), and polymeric $(\text{-PDI-X-})_n$ perylenediimide (PDI) derivatives as electron transport layer materials in p-i-n configured PSCs. It was revealed that macromolecular systems significantly outperform their small-molecule counterparts. The best devices employing polymeric ETLs achieved an efficiency of 16.4%, which is 2.2-fold higher than PSCs utilizing small-molecule PDI (7.6-7.8%). Dimeric PDI derivatives also demonstrated improved characteristics compared to monomers. These findings underscore the potential of polymeric and dimeric PDI as highly efficient non-fullerene ETLs.

Furthermore, the application of PDI derivatives as additives to enhance the morphology and reduce the defectiveness of PCBM films was investigated. While the incorporation of monomeric PDI into the ETL did not outperform pure PCBM in terms of efficiency, it also did not reduce device performance. However, composites incorporating polymeric PDI derivatives significantly enhanced the efficiency and stability of the solar cells. It is hypothesized that polymeric PDI act as linking agents, contributing to the formation of more homogeneous and less defective PCBM-based films, thereby explaining their superiority over monomeric analogues.

For n-i-p configured PSCs, the influence of the zinc oxide deposition method on the chemical composition of the ETL surface was studied. It was established that the traditional sol-gel method (based on zinc acetate) leads to the formation of residual CH_3COO groups on the ZnO surface, causing rapid degradation of $MAPbI_3$ perovskite. Conversely, the use of aqueous solutions of ammonia or methylamine enables effective passivation of the ZnO surface with amide end groups, significantly enhancing perovskite stability under prolonged light exposure.

Thus, a comprehensive approach to the development of novel ETLs and the optimization of their formation methods is crucial for achieving high efficiency and operational stability of perovskite solar cells.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (Project No. FFSG-2024-0008 / 124013000743-3).

Структура самособирающихся монослоёв на интерфейсах инвертированных перовскитных солнечных батарей

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Самособирающиеся монослои (SAM) широко используются для создания дырочно-транспортных слоёв перовскитных солнечных батарей. Их применение позволяет достигать хорошего согласования энергетических уровней с перовскитным абсорбером, снижения концентрации ловушек носителей заряда на интерфейсах, а также модулировать динамику кристаллизации перовскита [1]. 4-(3,6-диметил-9H-карбазол-9-ил)бутил]фосфоновая кислота (Me-4PACz) является наиболее широко используемой. Но её карбазольный фрагмент проявляет ограниченную эффективность: слабая способность фосфатных групп к закреплению на поверхности NiOx способствует образованию димеров и олигомеров, что приводит к их агломерации [2]. Сканирующая ближнепольная ИК-микроскопия демонстрирует, что соосаждение Me-4PACz с SAM на основе тиолов, в том числе 2-меркаптоэтанолом (ME), 3-меркаптопропионовой кислотой (MPA) и (3-меркаптопропил) триметоксисиланом (MPTMS) приводит к образованию гибридных монослоёв, формирующих плотное и однородное покрытие на поверхности NiOx. Островковая морфология гибридных SAM действует как шаблон для формирования объемного гетероперехода в перовскитном абсорбере, состоящего из взаимопроникающих доменов, богатых MA и FA катионами. Такая структура способствует эффективной генерации заряда, одновременно подавляя бимолекулярную рекомбинацию, тем самым повышая стойкость перовскитного абсорбера к деградации, вызванной электрическим полем [3].

Работа поддержана Российским научным фондом, проект No. 19-73-30020P.

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3. S. Cao et al. Hybrid Self-Assembled Molecular Interlayers for Efficient and Stable Inverted Perovskite Solar Cells. Adv. Energy Mater. 2025, 2405367.

Многоуровневый анализ радиационных эффектов в гибридных перовскитах: от эксперимента к моделированию

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Исследование транспортных слоёв на основе SnO_2 для гибких перовскитных солнечных элементов, изготовленных методом слот-дай нанесения

Асхат Нурканатович Жумабеков

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Детектирование фотоиндуцированных процессов в перовскитных солнечных элементах

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Композиты на основе углеродных нанотрубок и полианилинов как материалы для органической электроники и аккумуляторов

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Контакты в устройствах органической электроники

Дмитрий Юрьевич Паращук

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Мониторинг телеметрической информации как способ исследования свойств перспективных фотопреобразователей

Сергей Вячеславович Пушко

Российская аэрокосмическая компания “КБ1440”

Перспективы использования органических и перовскитных солнечных батарей в космосе

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Perovskite photovoltaics for solar-to-hydrogen production

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To date, research in the field of photovoltaics for solar-to-hydrogen (STH) production has been focused on developing highly efficient, scalable, and cost-effective devices. The solar-driven sub-module must generate the appropriate photo-potential to meet the thermodynamic and kinetic requirements for the water-splitting reaction. Crystalline silicon (c-Si), CIGS, and perovskite solar cells (PSCs) [1] are potential candidates for this purpose, with PSCs showing great promise due to their high photo-potential under solar illumination. Notably, PSCs exhibit superior performance under low light conditions without significant reduction in power conversion efficiency and open circuit voltage [2], making them particularly suitable for stable STH production systems.

Efficient water splitting relies on the use of electrodes in the electrolyzer, and the choice of electrode materials plays a crucial role in enhancing STH production efficiency. While noble-metal electrodes such as Pt, RuO_2, and IrO_2 are excellent catalysts, their high cost and limited availability hinder their widespread adoption. One conventional method to enhance the reactivity of pure metal catalysts is through alloying with other transition metals [3]. Alloying alters the bonding geometries of adsorbents and modifies the electronic structure of the pure metal surface.

In this study, we present the development of a stable and scalable PV-electrolysis system for water splitting, comprised of a PSC module and bifunctional catalytic electrodes based on nanoporous transition metal alloys. We prepared and evaluated the performance of a PSC sub-module, consisting of two PSCs with the following cell architecture: glass/FTO/TiO_2/$CH_3NH_3PbI_3[Pb(SCN)_2]$/spiroMeOTAD/Au, connected in series. Additionally, we synthesized and examined the properties of a number of electrode materials which were utilized as bifunctional electrocatalytic electrodes in the STH system, including NiCoPt/Graphene-dot catalyst with low Pt loading and Pt-free Ni@C core-shell nanoparticles [4].

The constructed electrolyzer based on the bifunctional Ni@C catalyst required approximately 1.5 V to operate, while the voltage from the two connected PSCs in series was nearly 2 V. The STH system demonstrated a water splitting efficiency of 8.5% under AM1.5G illumination (1000 W/m^2). Stability tests conducted under variable illumination intensities ranging from 10 to 1000 W/m^2 confirmed the reliability of the achieved STH efficiencies.

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Poster Presentations

Intrinsic stability challenges in design of absorber materials for lead halide perovskite solar cells

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We report the first systematic assessment of intrinsic thermal and photochemical stability of a large panel of complex lead halides $APbX_3$ incorporating different univalent cations ($A=CH_3NH_3^+$, $[NH_2CHNH_2]^+$, Cs^+) and halogen anions (X=Br, I) using a series of complementary analytical techniques such as UV-vis spectroscopy, x-ray diffraction, x-ray photoelectron spectroscopy, EDX chemical analysis, atomic force and scanning electron microscopy, electron spin resonance spectroscopy and mass spectrometry. We show that both heat stress and light soaking can induce a severe degradation of perovskite films even under well-controlled inert atmosphere in the absence of oxygen and moisture. The stability of complex lead halides increases in the order $MAPbBr_3<MAPbI_3<FAPbI_3<FAPbBr_3<CsPbI_3<CsPbBr_3$, thus featuring all-inorganic perovskites as the most promising absorbers for stable perovskite solar cells.
An important correlation was found between the stability of the complex lead halides and the volatility of univalent cation halides (AX) incorporated in their structure. In particular, $MAPbBr_3$ has the lowest stability since it is comprised of $PbBr_2$ and the most volatile MABr. On the contrary, all-inorganic $CsPbX_3$ compounds show remarkable stability since CsBr and CsI are non-volatile under the solar cell operation conditions. The established relationship provides useful guidelines for designing new complex metal halides with immensely improved stability.

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Fullerene-Based Interface Passivation Coatings for n-i-p Perovskite Solar Cells

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Perovskite solar cells (PSCs) have become a highly promising photovoltaic technology, offering power conversion efficiencies (PCE) on par with conventional silicon-based solar cells, along with the advantages of low-cost, solution-processable fabrication. In n-i-p device configurations, the electron-transport layer (ETL) is essential for efficient charge extraction and transport, directly affecting critical performance metrics such as open-circuit voltage, fill factor, and device stability. Thus, selection of the optimal ETL— considering factors like energy level alignment, charge carrier mobility, and interfacial defect passivation—is key to achieving high PSC efficiency and long-term reliability.

In this work, we present the synthesis of novel fullerene derivatives functionalized with hydroxyl and carboxyl groups, designed to passivate ITO and SnO_2 surfaces [1]. By comparing five fullerene derivatives as passivation layers, we identified a correlation between their molecular structure and PSC performance. Additionally, the introduction of an optimized passivation interlayer using a monocyclopropanated fullerene derivative with a carboxylic acid group significantly enhanced the device performance as compared to the reference PCBA-based devices. This research highlights the critical importance of tailored molecular design of fullerene-based SAM ETLs for improving charge extraction in n-i-p PSCs.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (Project No. 0089-2019-0010/AAAA-A19–119071190044-3).

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Структура самособирающихся монослоёв на интерфейсах инвертированных перовскитных солнечных батарей

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Thin reduced graphene oxide based films for nanoelectronics and sensors

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Flexible and organic electronics are becoming an increasingly popular field of science and technology due to the wide possibilities for integration into new wearable electronic devices, wide possibilities for creating new sensors, as well as radiation-resistant devices for space exploration. One of the promising classes of materials used in flexible and organic electronics are graphene derivatives, in particular graphene oxide (GO) and reduced graphene oxide (RGO).

To create electronic devices based on graphene derivatives, a method is required that allows controlling the electrical properties of the formed films by changing the number of functional groups on their surface, which in turn leads to a change in the band gap in these materials. There are various methods for reducing GO, but the most promising for local modification is the use of lasers.

In this study, a laser with a wavelength of 405 nm was used. The GO film on the surface of PET substrates was formed by spin coating (100 µL, 1000 rpm). It should be noted that at low fluence values of about 24 mJ/cm^2, the presence of a peak at ~1730 cm-1 is observed in the Fourier-IR spectra, which indicates the presence of carboxyl and carbonyl functional, which is important for sensorics tasks, since it allows binding various small organic and biomolecules to rGO. At the same time, a diffuse 2D peak containing various overtones is observed in the Raman spectrum, which indicates a low structuring of the film. Raman spectra for GO films reduced at 48 mJ/cm^2 fluence indicates an increase in the intensity of the 2D peak (~ 2700 cm-1), as well as a decrease in the resistance of the film. At a fluence of more than 60 mJ/cm^2, significant deformation of the GO film is observed, which indicates overheating of the film.

We used two abovementioned fluence parameters for formation of a sensitive area (24 mJ/cm^2) and contacts (48 mJ/cm^2) of a biosensor with further immoblisation of amine-modified thrombin aptamer Am-TBA with the nucleotide sequence 5'-GGTTGGTGTGGTTGG-3' which showed selective response on thrombin protein with detectable concentrations in range from 0,1 µM to 5 µM and fast response time in range from 35 to ~80 seconds.

Dopant-free polymeric hole-transport materials for perovskite solar cells: simple is best!

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A series of (BDD-X)$_n$ conjugated polymers comprised of 5,7-bis(2-ethylhexyl)benzo[1,2-c:4,5-c′]dithiophene-4,8-dione (BDD) and X = B (**P1**), X = TBT (**P2**) and X = TBTBT (**P3**), where T = thiophene, B = benzo[c][1,2,5]thiadiazole, have been synthesized and applied as dopant-free hole-transport layer materials in perovskite solar cells (PSCs). We explored the effect of the molecular structure of the block X on the optical and electronic properties of the polymers, nanoscale morphology of their films, and the impact of all these parameters on the performance of the polymers in PSCs. As a result, using the polymer **P1** with the simplest molecular architecture provided the power conversion efficiency (PCE) of 20.1% in solar cells thus outperforming the devices assembled with more sophisticated polymers **P2-P3** or the reference poly(triarylamine)-based hole-transport materials. The enhanced device performance is attributed to a better HOMO alignment of **P1** with respect to the perovskite valence band, low concentration of defects and suppressed carrier recombination at **P1**/perovskite interface and, most importantly, highly uniform film structure as revealed by atomic force microscopy and infrared scattering near-field optical microscopy (IR s-SNOM) techniques. The supramolecular interactions of the building blocks of polymers **P1-P3** with the perovskite films resulting in the passivation of surface defects were further studied by density functional theory calculations.

This work was supported by the Russian Science Foundation (projects No. 23-73-01196).

Синтез поликарбоксильных производных фуллерена – перспективных материалов самоорганизующихся монослоев n-типа для перовскитных солнечных батарей

Е.А. Кулябина[1,2], В.С. Большакова[1], А.С. Перегудов[3], О.А.Краевая[1], П.А.Трошин [4,1]

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Производные фуллеренов активно применяются в перовскитных солнечных батареях как электрон-транспортные материалы, благодаря своей высокой подвижности электронов и хорошему согласованию энергетических уровней с валентной зоной и зоной проводимости перовскитных материалов. Поликарбоксильные производные являются перспективным классом соединений для формирования самоорганизующихся монослоев (SAMs) n-типа. Наличие нескольких карбоксильных групп обеспечивает прочное закрепление молекул на поверхности оксида металла, способствуя формированию плотного монослоя, что позволяет эффективно пассивировать поверхностные дефекты, уменьшая рекомбинацию зарядов.

Синтез поликарбоксильных производных C_{60} и C_{70} осуществляется посредством функционализации фуллеренового каркаса путем присоединения атомов хлора с последующим замещением их на метиловые эфиры гидрокоричной кислоты и гидролизом эфирных групп [1]. Синтез амидных производных предполагает получение триметилсиллилового эфира аминокислоты и его последующее добавление к хлорангидриду фуллереновой кислоты, образующегося *in situ* [2]. Нами было синтезировано шесть новых поликарбоксильных производных фуллерена C_{60} и C_{70} (схема 1), их состав и строение были подтверждены с использованием спектроскопии ЯМР и МАЛДИ масс-спектрометрии. Планируется исследование полученных материалов в качестве самоорганизующихся монослоев n-типа в перовскитных солнечных батареях.

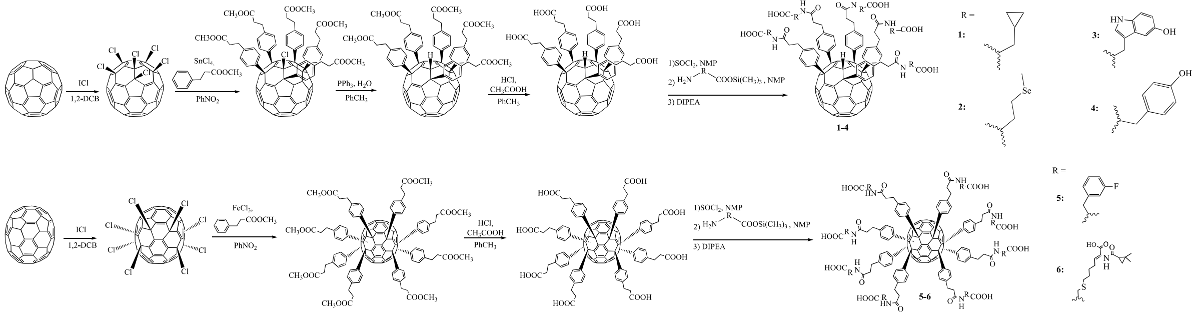

Схема 1. Синтез поликарбоксильных производных фуллерена C_{60} и C_{70}

Работа поддержана проектом Министерства науки и высшего образования Российской Федерации № FFSG-2024-0008 (124013000743-3)

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Radiation hardness assessment of organic semiconductors

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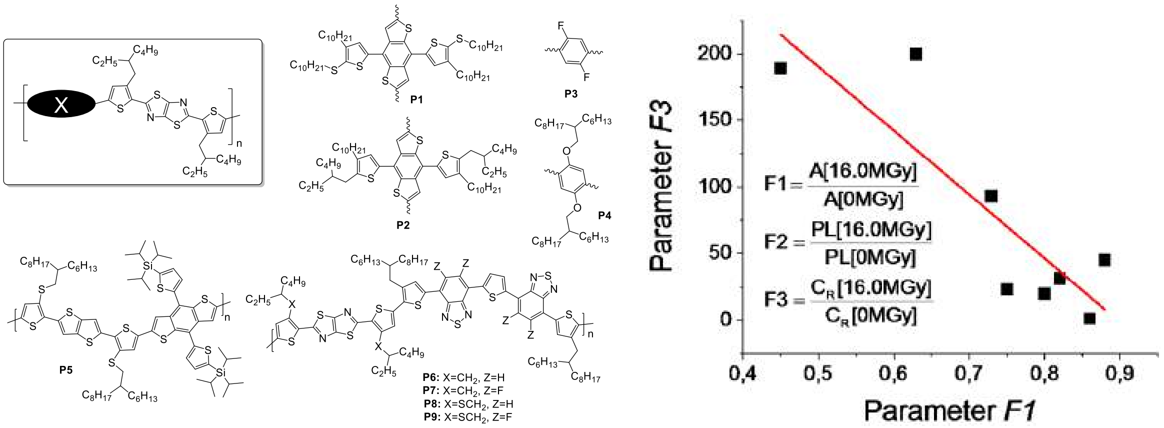

Figure 1. Molecular structures of the studied model polymers **P1-P9**

We have designed and presented here a possible research methodology for the systematic screening and assessment of the radiation hardness of organic semiconductors. We propose to use three indices, each based on one type of spectral data (Fig. 1b). First, we have compared the absorption of the semiconductor film before and after irradiation, which gives us the parameter F1 (Eq. 1, Fig. 1b): the lower its value, the less stable is the material. Similarly, the parameter F2 (Eq. 2, Fig. 1b) is based on the comparison of the radiation intensity of the polymer thin films before and after irradiation, so higher F2 values indicate a reduced susceptibility to radiation-induced defects and, therefore, a higher stability of the material. The parameter F3 (Eq. 3, Fig. 4) reflects the accumulation of radicals in the material after radiation irradiation. Parameter F2 does not correlate well with two other parameters. Most probably, this is due to very deep quenching of the photoluminescence of polymer films after receiving a huge dose of radiation (16 MGy): emission is almost absent for all the samples except **P5** and **P4**. Therefore, it may be recommended for future studies to determine F2 value for samples that received a smaller dose of gamma rays, e.g., 1-5 MGy instead of 16 MGy. Parameters F1 and F3 show quite a decent correlation with each other if we exclude from consideration the extremely high value suspiciously obtained for **P6**. The correlation could be fitted with a linear equation with the Pearson's correlation coefficient r = 0.86 (Fig. 4). This finding suggests that both F1 and F3 provide rather adequate benchmarking of the radiation hardness of the polymers P1-P9. Very exciting was the observation that polymers **P1-P9**, being good representatives of organic semiconductors, have demonstrated higher radiation hardness than the vast majority of the commodity-type non-conjugated polymers, such as polypropylene, PET, PVDF, etc. This finding points to the bright future of organic semiconductors in the design of a new generation of electronics with supreme radiation hardness for application in harsh aerospace or terrestrial environments.

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Design of PV-grade functional materials for perovskite solar cells

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Perovskite solar cells (PSCs) have attracted significant attention from the scientific community due to their remarkable progress in power conversion efficiency (PCE). Since their initial report in 2009 with a PCE of 3.8%, their performance has rapidly advanced, surpassing 26% by 2025. PSCs now outperform various established photovoltaic technologies, including organic, thin-film chalcogenide, amorphous silicon, and multicrystalline silicon solar cells, and are approaching the efficiency levels of crystalline silicon-based photovoltaics. [1,2]. Perovskite-type semiconductors exhibit a unique combination of solution processability with exceptional defect tolerance, coupled with highly tunable bandgaps, large extinction coefficients, and long charge carrier diffusion lengths.[1-3]. The high efficiency and potential for low-cost production of PSCs highlight their significant commercial promise as an emerging photovoltaic technology. However, their widespread adoption is currently hindered by stability-related challenges. Addressing these limitations through the development of novel advanced materials and optimized fabrication techniques represents a key pathway toward their successful commercializations.

In this presentation, we report on the results of a long-term collaborative effort between FOMaterials Ltd. and the FRC PCP RAS. Our joint work has been focused on the development of a comprehensive set of key functional materials for PSCs. Starting ten years ago with the synthesis of high-purity, photovoltaic-grade precursor materials such as PbI_2, MAI, and FAI, the collaboration has since progressed to the design and optimization of advanced charge-transport materials. Notably, we have developed novel polymer-based hole-transport materials and fullerene-based electron-transport materials, which have enabled significant improvements in both device performance and operational stability. State-of-the-art PSCs fabricated using these materials demonstrate power conversion efficiencies more than 24% under standard test conditions, marking a substantial step toward their practical implementation [4-13]. While being the exclusive supplier of FRC PCP MC RAS within a half of the decade, FOMaterials also emerged as the leading producer of organic and perovskite PV materials within Russia. At the current stage, we are looking for an extension of our network of collaborations and supporting global research activities focused on the development and commercialization of organic and perovskite PV technologies.

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Boosting Perovskite Stability: Azaadamantane Derivatives as Advanced Multifunctional Additives

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Complex lead halides incorporating simultaneously a few univalent cations such as cesium (Cs^+), methylammonoium (MA^+) and formamidinium (FA^+) represent highly promising materials for perovskite solar cells delivering record-high power conversion efficiencies. Unfortunately, these materials demonstrate insufficient stability, which limits their practical implementation; therefore, improving the photochemical and thermal stability of multication lead halide perovskites is an urgent task, which needs to be addressed to achieve sufficiently long operational lifetimes of perovskite solar cells which are required for their massive real-life applications.

Herein, we present a comparative study of two azaadamantane-based molecular modifiers as stabilizing additives for $Cs_{0.10}MA_{0.15}FA_{0.75}PbI_3$ and $Cs_{0.12}FA_{0.88}PbI_3$ perovskite formulations. An iodide of N-methylated 1,3,5,7-tetraazaadamantane known as urotropine (MAdI) showed a modest stabilizing effect reflected in a decreased amount of PbI_2 formed as the decomposition product from $Cs_{0.10}MA_{0.15}FA_{0.75}PbI_3$ and suppressed light-induced crystallization of $Cs_{0.12}FA_{0.88}PbI_3$. On the contrary, 4,6,10-trihydroxy-3,5,7-trimethyl-1,4,6,10-tetraazaadamantane hydrochloride (NAdCl) strongly enhanced the stability of both lead halide perovskites and prevented the formation of metallic lead Pb^0 as a photolysis product. Different stabilizing effects caused by MAdI and NAdCl were related to their different localization within the perovskite films as evidenced by nanoscale infrared (IR) s-SNOM microscopy.

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Design, synthesis, and structure-property relationship study of new push-pull fused oligomers based on indolo[3,2-b]indole and benzothieno[3,2-b]benzothiophene

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

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

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

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

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Polymer photovoltaic materials based on three-component composites containing fullerenes and phthalocyanine derivatives

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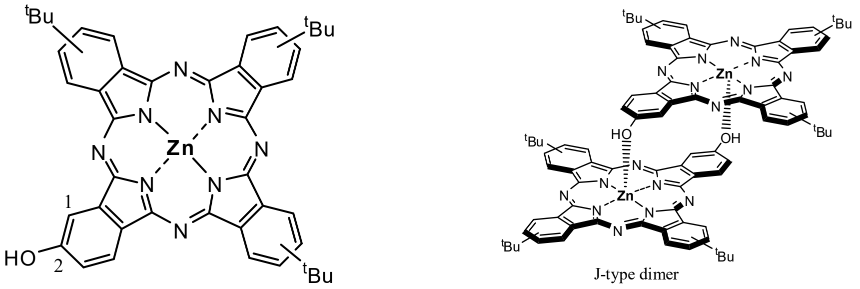
Three-component composites [poly(3-hexylthiophene) (P3HT) - C_{60} – mono/dimeric zinc phthalocyanine complex] were used to assemble photovoltaic cells. The photovoltaic properties were investigated on model solar cells where we are using the already known bulk hetero-junction concept as an active layer which consists of a mixture of monomer **I** or dimer **II**, (fig.1) fullerene (C_{60}) and the well-known polymer P3HT. [1, 2]



(I) (II)

Fig. 1. Monomer **I** and dimeric phthalocyanine zinc complex of 2-hydroxy-9(10),16(17),23(24)-tri-tert-butylphthalocyanine

Previously, sensitization of the internal photoelectric effect was detected during irradiation of PCM (MEH-PPV/C_{60}-MPc) in the near IR region, which is explained by photogeneration of charge carriers from phthalocyanine molecules. It was shown that in bulk-heterojunction photovoltaic converters (PVC) based on PCM (MEH-PPV/C_{60}-PcBuZn), the photoconductivity current density increases by an order of magnitude compared to PVC based on PCM (MEH-PPV/C60).[3] In order to increase the conversion efficiency of solar cells by increasing absorption in the near IR region, PCMs containing $ZnPc(t\text{-}Bt)_4$ or the dimer $ZnPc(t\text{-}Bt)_3(OH)$ with an absorption maximum in the spectral region greater than 700 nm were studied.

The photovoltaic properties of three-component composites of P3HT, C_{60}, and phthalocyanine complexes **I** or **II** were studied. The experimental data obtained in this work show that monomer **I** and the dimer **II** zinc phthalocyanine complex are of interest for further investigations since they are promising compounds for use as materials in photovoltaic devices.

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Design of triphenylamine-based molecules with anchor group for interfacial layers of perovskite solar cells

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Perovskite solar cells (PSCs) are a rapidly evolving technology, with their efficiency soaring from 3.8% in 2009 to over 25% by 2025, allowing them to compete with and even outperform traditional silicon solar cells in laboratory conditions [1]. These characteristics, combined with low-cost materials and ergonomic manufacturing methods, have made PSCs a promising photovoltaic technology. A major problem standing in the way of commercialization and scaling of PSCs is their low stability, as well as degradation during operation of the device. The solution to this problem is the use of auxiliary layers in the PSC architecture, the so-called interface layers based on organic semiconductor materials. The feature that allows such materials to effectively "treat" defects in the perovskite structure is the presence of special functional groups (anchor groups) capable of specific interactions with the perovskite material and other charge-transport layers, as well as of self-assembly. However, the variety of possible surface and volume defects in perovskite, leads to the problem of finding optimal structure of the self-assembled materials. An important part of these materials is the terminal group, which is oriented toward the perovskite layer and responsible for specific interactions with the active layer. In addition, the terminal group affects the surface properties of the film formed by the material; the combination of all properties, including optical, electrochemical, etc., has a significant impact on the efficiency and stability of PSCs and perovskite solar modules (PSMs), as we have shown previously [2,3]. Nevertheless, the selection of structural blocks for this group, as well as the search for optimal substituents in it, is currently an unexplored area of scientific knowledge.

In this work, a comprehensive study is conducted to identify a number of patterns of influence of substituents at the terminal group on the properties of compounds. For this purpose, an effective scheme of the synthetic route of a series of compounds differing in the substituent at the terminal group was developed, a set of their physicochemical properties (such as optical and electrochemical properties, thermal stability and phase behavior) was studied. The surface properties of films formed by the materials were investigated, and the influence of substituents and their donor-acceptor nature on the complex of properties of the obtained compounds was revealed. The possibility of using these materials in PSCs was assessed – for all materials, efficiency indicators of more than 20% and good stability were achieved.

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

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Stability assessment of organic solar cells under exposure to different types of ionizing radiation

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In recent years, significant progress has been made in improving the power conversion efficiency (PCE) of organic solar cells (OSCs) that is coming close to 20% now. [1] OSCs on flexible plastic substrates have attracted particular attention due to their multiple advantages, such as compatibility with the high-throughput roll-to-roll production process, lightweight design, mechanical flexibility, and the potential for large-scale production. [2] High specific power of up to 40 W g^{-1} reached for organic solar cells in combination with unique mechanical characteristics makes promising their application in space missions. Therefore, one of the main issues defining the suitability of OSCs for space applications is their stability under the influence of cosmic radiation.

This paper presents the results of our systematic study on the resistance of OSCs to several types of ionizing radiation. The obtained results confirm that organic solar cells can tolerate quite significant doses of radiation. In particular, they withstand 20 kGy dose of γ-rays without any significant change in the efficiency. The exposure to high-energy electrons (8.5-10 MeV) with a fluence of 10^{14} e/cm^2 causes the decrease in the device PCE by ca. 30% from the initial value. Comparable aging effects were observed after device exposure to accelerated protons (18 MeV) with a fluence of 10^{13} p/cm^2. Oit should be emphasized that the corresponding doses of radiation are accumulated in the low earth orbit (LEO, International Space Station orbit) within several decades. Furthermore, we have revealed a clear "self-healing" effect of OSCs after radiation exposure, which should substantially increase their lifetime in space. Thus, the obtained results confirm exceptionally high potential of organic solar cells as an emerging PV technology for space applications.

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

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Synthesis of polymers based on triphenylamine with fluorinated and cyanocontaining electron-withdrawing groups

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Currently a wide range of organic hole-transport materials based on triphenylamine (TPA) derivatives, which are important components of organic electronics and photonics devices, have been developed. Among them special attention is paid to polymers [1, 2], since compared with low molecular weight compounds TPA-based polymers have better thermal stability, good film-forming properties, and improved adhesion to the substrate.

The optoelectronic properties of conjugated polymers can be effectively controlled by intramolecular charge transfer via donor–acceptor (D-A) interactions [3, 4]. The introduction of electron-withdrawing groups makes it possible to change the light absorption region, vary the energy of the HOMO and LUMO levels, and reduce the band gap of hole-transport materials.

The currently known examples of D-A polymers based on triphenylamine, as a rule, are obtained by cross-coupling reactions using expensive catalysts [4]. The simplest method for synthesizing such polymers is oxidative polymerization with $FeCl_3$ [3].

In this work, D-A polymers based on TPA were obtained by oxidative polymerization with $FeCl_3$ (Fig. 1). The properties of the obtained compounds were studied. The data obtained in the study of polymers as hole-transport layers of perovskite solar cells are presented.

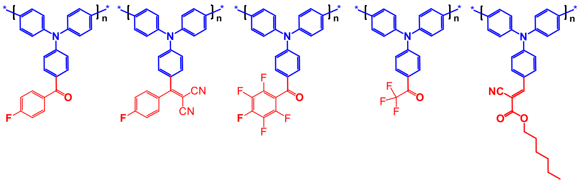

Figure 1 - Structural formulas of D-A homopolymers

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Investigation of mechanisms for forming uniform gel-polymer electrolyte layers

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Gel-polymer electrolytes (GPEs) are promising functional materials combining the advantages of solid and liquid electrolyte systems, including high ionic conductivity, mechanical stability, and enhanced operational safety. Due to their unique combination of physicochemical properties, GPEs possess significant potential for application in a wide range of electrochemical devices, such as lithium-ion batteries, supercapacitors, electroanalytical sensors, electrochromic systems, and physiological parameter monitoring devices. A critical factor in the design of such devices is ensuring uniform deposition of functional layers, which is essential for stable and accurate performance of GPE electrolyte layers.

Liquid-phase deposition is the dominant methodological approach for forming thin-film polymeric structures, including methods such as inkjet printing, slot-die coating, spray coating, and other specialized deposition methods. A significant limiting factor in achieving uniform layers through liquid-phase deposition is the coffee ring effect (CRE), which occurs during solvent evaporation. This phenomenon involves the migration of dissolved or dispersed particles in an evaporating liquid to the droplet periphery, forming characteristic ring-shaped deposits, leading to non-uniform material distribution and, consequently, spatial anisotropy in ionic conductivity within the GPE layer. The drying of applied inks, which forms a dry deposit, is a critical stage influencing the morphology of printed structures. The final profile of the resulting deposits is determined by the properties of the inks and the drying conditions. Understanding and controlling this process are crucial for ensuring the specified functional properties of structures obtained via liquid-phase deposition. This study investigates the deposition mechanisms of lignin-based gel polymer electrolyte (GPE) solution using dimethyl sulfoxide (DMSO) as the main solvent and glycerol (10 vol. %) as a co-solvent to suppress the coffee ring effect (CRE).

The results of studying the dynamics of sessile droplet evaporation at different temperatures revealed key patterns of deposit formation. It was shown that the addition of 10 vol. % glycerol as a co-solvent is an effective strategy for suppressing the coffee ring effect. This approach regulates viscosity and creates a surface tension gradient, leading to a significant suppression of the CRE. So, the coffee ring index (CRI) increased from 0.27 (pure DMSO) to 0.51 (DMSO-glycerol) at 90 °C, with optimal homogeneity already achieved at 70 °C. Modeling of internal Marangoni flows and radial capillary flows revealed their mutual influence on the formation of final deposit profiles. It was found that the balance of these flows plays a decisive role in ensuring uniform distribution of the material during solvent evaporation. Mathematical description of the radial distribution of the polymer concentration on the droplet surface taking into account the evaporation flow profile allowed a deeper understanding of the physical processes underlying the formation of inhomogeneities. The obtained results are of great practical importance for the development and optimization of production technologies for various electrochemical devices.

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Молекулярные модификаторы для повышения фотостабильности перовскитных солнечных элементов на основе $CsPbI_2Br$

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Низкая эксплуатационная стабильность гибридных перовскитных солнечных элементов в настоящее время является основным препятствием для их практического внедрения. Замена органических фрагментов неорганическими катионами представляет собой многообещающий подход к созданию более стабильных поглощающих материалов. Неорганические перовскиты на основе галогенидов свинца $CsPbI_{3-x}Br_x$ (x=0-3) продемонстрировали улучшенную термическую и фотохимическую стабильность. Среди них $CsPbI_2Br$ считается наиболее перспективным фотоактивным материалом из-за оптимальной комбинации фазовой стабильности и ширины запрещенной зоны.

Мы предложили группу перспективных модификаторов, эффективно подавляющих фазовые превращения в пленках $CsPbI_2Br$ в течение более чем 10 000 ч при непрерывном облучении светом, а также при воздействии гамма-излучения (изотопный источник ^{60}Co).

Сравнительный анализ стабилизирующих эффектов структурно близких модификаторов выявил преимущество добавок с двумя катионными центрами, что может быть объяснено более высокой структурной стабильностью перовскитных материалов со структурным типом Диона-Якобсона, за счет более коротких межслоевых расстояний по сравнению с их аналогами, образующими структуры Раддлесдена-Поппера.

Обнаружено, что наличие в модификаторе длинных алкильных заместителей способствует более быстрой деградации при облучении гамма-излучением, вероятно за счет образования дополнительных радикалов. Солнечные элементы с наиболее эффективными стабилизирующими агентами позволили сохранить более 90% первоначального КПД после облучения гамма-лучами с суммарной дозой 1300 кГр, а также улучшенной эксплуатационной стабильностью при облучении солнечным светом.

Работа выполнена при поддержке Российского научного фонда (проект 22-13-00463-П).

Stabilizing $CsPbI_2Br$ against Halide Segregation via Doping: A Route to Improved Radiation and Light Tolerance

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All-inorganic perovskite materials, such as $CsPbX_3$ (X = I, Br), have garnered significant attention due to their chemical robustness and optoelectronic properties, enabling high power conversion efficiencies (PCE) in solar cells. Among these, $CsPbI_2Br$, achieved through partial substitution of iodide with bromide ion, offers an optimal balance between bandgap (1.92 eV) and stability, making it suitable for optoelectronic applications, including tandem solar cells. However, $CsPbI_2Br$ is prone to light-induced halide segregation, leading to the formation of bromide-rich and iodide-rich domains. This issue can be mitigated by incorporating organic passivation molecules, such as crown ethers, ammonium salts, and amino acids. While these strategies have achieved PCEs of over 17%, they compromise the thermal and chemical stability of all-inorganic perovskites, limiting their operational stability in tandem configurations with silicon or CIGS technologies. Alternative approaches, such as B-site modification (partial substitution of Pb^{2+}), have also demonstrated effectiveness.

Despite significant progress, a comprehensive understanding of the relationship between substituent cation types and their impact on device efficiency and stability remains lacking. This study systematically investigates the partial substitution of Pb^{2+} in $CsPbI_2Br$ with a wide range of metal cations, focusing on their effects on photostability, radiation robustness, and resistance to halide phase segregation.

A series of $CsPb_{0.95}M_{0.1/n}Br$ systems, involving 30 different substituent cations M^{n+}, was examined. The results demonstrate that light-induced phase segregation can be effectively suppressed through appropriate compositional engineering. Additionally, the incorporation of certain cations significantly enhances radiation stability, a critical factor for applications in harsh environments, such as space or high-energy radiation settings. This study provides valuable insights into optimizing the performance and durability of all-inorganic perovskites for advanced optoelectronic applications.

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