ANNOTATION

Dissertations for the degree of Doctor of Philosophy (PhD)
8D05302 - Physics

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Structural, optical and electrical transport properties of PEDOT:PSS films in polymer solar cells

Topic relevance. Currently, the greatest interest among various scientific international communities is caused by inexpensive, environmentally friendly and flexible organic solar photoconverters, the efficiency of which already exceeds 14% even for a simple architecture with one active layer and two components. The development of such OSCs is essential to preserve the global environment and ensure sustainable economic growth.

The design of a typical solar cell is a photoactive layer in which electron-donor and acceptor materials are placed in a single layer, forming a bulk heterojunction, which promotes the dissociation of excitons into free charges. To reduce charge recombination at the interfaces and increase the efficiency of charge injection, the photoactive layer is placed between the electron and hole transport layers (ETL and HTL, respectively).

The performance of organic photoconverters is highly dependent on the quality of the ETL and HTL transport layers. Strict requirements are placed on their functional properties, such as flexibility, low series resistance, high light transmittance in the visible light range and thermal stability. Inorganic transition metal oxides have become widely used as HTL materials for OSCs. However, the use of vacuum deposition and vapor deposition technology is an expensive process, so this limits their use. At present, significant efforts of specialized laboratories in the world are aimed at finding relatively cheap mass-produced, transparent in the visible region of the spectrum, and thermally stable conductive materials. Among the currently available HTL materials for organic photoconverters, the composite of poly(3,4-ethylenedioxythiophene) and polystyrene sulfonate (PEDOT:PSS) stands out due to its ease of processing, low cost, non-toxicity, and chemical stability.

At the same time, the presence of bulk and surface defects near the PEDOT:PSS/photoactive layer interface is one of the reasons for the poor performance of OSCs. This leads to an increase in charge recombination at the interface, a deterioration in the transport of holes, and a decrease in the efficiency of hole extraction by the electrode. To solve these problems, various bulk and surface modifications of PEDOT:PSS are currently being used using solvents, surfactants, acids, and various additives. This helps optimize the structure and electrical properties of PEDOT:PSS films, improve interlayer contact, and improve OSC stability and performance.

The dissertation aim is to study the effect of modification of the structure of PEDOT:PSS films on the photovoltaic characteristics of polymer solar cells.

The objects of research are PEDOT:PSS films, nanobelts of phthalocyanine and its metal complexes, tungsten disulfide nanoparticles, polymer solar cells.

The scientific novelty consists of the following:

1. The influence of the boiling point of alcohols on the weakening of bonds between PEDOT and PSS has been established. It is shown that, depending on the boiling point of alcohols, homogeneous PEDOT:PSS films with a low degree of roughness, improved bulk conductivity, and low transition resistance at the interface with the photoactive layer are formed.
2. The role of thermal annealing in the process of PEDOT:PSS film formation is determined. It is shown that thermal annealing leads to a smoothing of the surface interface and a decrease in the intensity of the absorption spectrum of the PSS aromatic fragment. It has been established that thermal annealing leads to a decrease in the film resistance and an increase in the charge injection efficiency, efficiency, and quantum efficiency of the OSC.
3. It has been established that the admixture of MPc nanobelts in a PEDOT:PSS film contributes to a decrease in roughness and an increase in the degree of crystallization of the film. It is shown that doping PEDOT:PSS with MPc nanobelts leads to a decrease in the series resistance and an increase in the OSC efficiency.
4. The influence of WS_2 nanoparticles on the injection and transport of charge carriers in PEDOT:PSS has been established. It is shown that impurities of WS_2 nanoparticles contribute to a decrease in surface defects in the film, a decrease in the interfacial resistance of charge carriers transfer, and an increase in the efficiency of the OSC.

The structure and scope of the dissertation. The structure of the dissertation work is determined by the tasks set and consists of an introduction, 4 sections, a conclusion, a bibliography and an appendix. It is presented on 103 pages of typewritten text, illustrated with 47 figures, 17 tables, contains a list of references from 231 titles.

The main results include the following:

1. Alcohol solvents and thermal annealing prevent the formation of PSS-riched agglomerates, which leads to improved hole transport at the PEDOT:PSS/photoactive layer and PEDOT:PSS/ITO interfaces.
2. The incorporation of phthalocyanine nanobelts and its metal complexes into the PEDOT:PSS hole-transport layer improves the crystallinity and reduces the film resistance.
3. There is a critical concentration of WS_2 nanoparticles in the PEDOT:PSS film, the excess of which leads to the ejection of nanoparticles to the surface of the film, as a result, a sharp increase in the interfacial resistance of the hole-transport layer is observed.

Scientific and practical significance of the work: a technology has been developed for obtaining a composite hole-transport electrode OSC based on

PEDOT:PSS with high stability and performance; the optimal parameters of an organic solar cell (structural features, production technology) are determined, which ensure a high efficiency and quantum efficiency. The results obtained can be used in the development of photovoltaic and optoelectronic cells, light emitting diodes, in flexible electronics and thermoelectric devices. This technology will have the prospect of creating light, technologically advanced and cheap in mass production autonomous power supply sources for a wide range of electronic equipment and devices.

Approbation of the work and publications. The main results of the work were reported and discussed at the conferences: VIII International Conference "Laser, Plasma Research and Technologies" LaPlaz-2022, dedicated to the 100th anniversary of the birth of the Nobel Prize winner in physics Nikolai Gennadievich Basov (Moscow, 2022); XI International Conference on Photonics and Information Optics (Moscow, 2022); XV International Scientific Conference "Physics of the Solid State" (Astana, 2022); IV International Scientific and Technical Conference "Minsk Scientific Readings-2021" (Minsk, 2021); 5th International Symposium on Molecular Photonics dedicated to the memory of Academician A.N. Terenin (1896–1967) (St. Petersburg, 2021); X International Conference on Photonics and Information Optics (Moscow, 2021); Republican scientific and practical online conference dedicated to the 85th anniversary of the prominent scientist, the first dean of the Faculty of Physics, Doctor of Pedagogical Sciences, Professor, Academician of the Academy of Pedagogical Sciences of Kazakhstan Aryngazin Kanapiya Mubarakovich (Karaganda, 2021); VII International Conference "Laser, Plasma Research and Technologies" LaPlaz-2021 (Moscow, 2021); International scientific and practical conference "Auezov readings - 18: the spiritual heritage of the great Abai" to the 175th anniversary of Abai Kunanbaev (Shymkent, 2020); The 8th International Conference on Nanomaterials and Advanced Energy Storage Systems INESS-2020 (Astana, 2020); International scientific and practical Internet conference "Innovative technologies in the system of physics and mathematics education" (Minsk, 2020).

Publications. According to the results of the dissertation work, 18 printed works were published: 3 articles in journals included in the Thomson Reuters and Scopus database (1 article in the J Polymers for Advanced Technologies, 2021, IF – 3.348, Q2, percentile 79; 1 article in the Optical Materials, 2022, IF – 3.754, Q2, percentile 71, 1 article in the Synthetic Metals, IF – 4.0, Q2, percentile 84); 4 articles in the journal recommended by the Committee for Control in the Sphere of Science and Higher Education of the MSHE RK and 11 publications in the materials of international conferences.