UDC 621.382 + 539.23
DOI https://doi.org/10.32782/2663-5941/2025.6.1/59

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ELECTROPHYSICAL PROPERTIES OF HETEROSTRUCTURES WITH PHTHALOCYANINE LAYERS FOR PHOTOVOLTAIC APPLICATIONS

The article investigates the electrophysical properties of heterostructures based on porous silicon with deposited layers of copper and lead phthalocyanines, which are promising organic materials for next-generation photovoltaics. The relevance of the study is driven by the search for inexpensive, flexible, and stable organic photoconverters capable of complementing or replacing traditional silicon solar cells. The porous layer was obtained using metal-assisted chemical etching, after which solutions of CuPc and PbPc in DMSO were applied to the prepared surface. The electrophysical characteristics were examined by impedance spectroscopy and DC I–V measurements.

It is shown that the heterostructures exhibit rectifying behavior; however, the conduction mechanisms strongly depend on the type of central metal in the macrocycle. For the por-Si/CuPc structure, three characteristic conduction regions were identified, corresponding to thermo–field emission, recombination processes in the space-charge region, and current limitation by the series resistance. In the case of por-Si/PbPc, the dominance of series resistance is observed already at ultralow voltages (above 0.006 V), indicating the formation of a high-resistance interface and poorer transport properties compared to CuPc.

Molecular modeling of CuPc and PbPc presented in the article showed that the lead complex is significantly non-planar due to the much larger ionic radius of Pb^{2+}, whereas CuPc retains a planar conformation. The non-planarity of PbPc leads to an increase in internal strain within the molecule and worsens energy alignment at the heterojunction, which correlates with the observed high value of series resistance. Analysis of the frequency dependence of conductivity confirmed the dominance of the drift mechanism of charge transport up to frequencies of 10^6 rad/s for both structures.

The obtained results demonstrate the critical role of the central metal in forming energy barriers and transport properties of por-Si/McPc heterostructures and identify CuPc as a more suitable material for developing efficient organic–inorganic photoconverters.

Key words: *metal–phthalocyanine films, macrocycle, organic heterojunction, porous silicon, I–V characteristics.*

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Formulation of the problem. Photovoltaics is one of the most promising areas of modern energy production, as it enables the generation of electricity from a constant and free energy source–the Sun. The use of solar panels makes it possible to increase the energy independence of portable devices, individual buildings, and even entire countries, while not polluting the environment. The main challenges of modern silicon photovoltaics, which dominates terrestrial applications, are related to the need to increase efficiency and reduce the production cost of solar cells in order to ultimately decrease the cost of 1 kWh of energy [1, p. 2].

In addition, a current societal demand is the development of lightweight and flexible photoconverters capable of powering wearable electronic devices [2]. Therefore, a clear shift has emerged in the field of photovoltaics–from monocrystalline silicon solar cells toward devices based on organic analogues. The use of organic materials in photovoltaic device fabrication makes it possible to significantly reduce the temperature of standard technological processes (vacuum technologies [3, p. 1735; 4, p. 2]), employ inexpensive synthesis methods (roll-to-roll printing, solution processing [5, p. 17]), broaden the absorption spectrum of solar radiation (due to the ability to modify chemical composition [6, p. 379]), enable the fabrication of flexible panel designs [5, p.10], and even achieve integration with textiles [7, p. 3872].

Thus, organic photovoltaic devices open up promising opportunities for the development of low-cost, lightweight, flexible, and spectrally adaptable solar energy systems.

Analysis of recent research and publications. Modern literature presents studies on various types of organic materials (electron donors and acceptors) for use in the active layer of organic solar cells, where light absorption, exciton generation, and their separation into free charge carriers occur, determining the energy conversion efficiency [5, p. 3]. In particular, the active layer of such a solar cell may include donor materials such as conjugated polymers [5, p. 7], merocyanines [8, p. 320], porphyrins [9, p. 20172], phthalocyanines [10, p. 2], or small donor–acceptor molecules [11, p. 4].

Among these, phthalocyanines represent one of the most promising classes of organic semiconductors for use in organic photovoltaic devices due to their relatively high thermal stability (they do not decompose at 300–400 °C), chemical stability (resistant to oxygen, moisture, etc.), and photostability (resistant to UV radiation) [12, p. 16; 13, p. 803]. In other words, unlike polymers, this material can significantly improve the stability of organic solar cells and, consequently, their service life, which is one of the main limitations of such devices.

Phthalocyanines are among the few organic materials well-suited for vacuum deposition, which ensures high-purity films, precise thickness control at the nanometer level, and the possibility of obtaining a crystalline structure [10, p. 5]. Polymeric materials, which are mostly processed using solution-based technologies, do not always provide such reproducibility in chemical composition and structure.

Moreover, phthalocyanines allow flexible modification of their energy levels by incorporating different central metals (Cu, Zn, Co, Fe, Pb) [14, p. 3], which determines their electrical and optical properties. Specifically, Cu-doped phthalocyanines have absorption maxima in the visible range, whereas Pb-doped phthalocyanines absorb in the infrared (IR) range, where most polymers do not [15, p. 6]. Clearly, combining both types of phthalocyanines can significantly broaden the spectral efficiency of such solar cells (from UV to IR). Additionally, different central atoms and synthesis conditions will provide varied electron transport characteristics [10, p. 4]. Therefore, establishing the influence of synthesis conditions and substrate type on the electrophysical properties of metal–phthalocyanine films requires more detailed investigation.

Task statement. The aim of the article is to investigate the electrophysical properties of metal phthalocyanine layers on porous silicon and to model the molecular structure of phthalocyanines in order to determine the charge transport mechanisms in organic–inorganic heterojunctions.

Outline of the main material of the study.

Sample preparation. The porous layer was formed using a two-step metal-assisted chemical etching method with the following solutions:

1. Silver deposition solution: 68 mg of silver nitrate ($AgNO_3$) was dissolved in 10 ml of distilled water, then 4.42 ml of 40% hydrofluoric acid (HF) was added, and the total volume was brought to 20 ml with distilled water.

2. Etching solution: 11 ml of 40% HF was added to 30 ml of distilled water, followed by the addition of hydrogen peroxide (H_2O_2), and the total volume was adjusted to 50 ml with distilled water.

The samples were immersed in the first solution for 20 or 40 seconds to deposit silver particles. Afterward, all wafers were rinsed with distilled water. Both groups of samples were then transferred to the second solution for etching for 45 minutes. After etching, the wafers were immediately rinsed with distilled water

and dried in a centrifuge. The formation of porous silicon was visually confirmed by the characteristic red photoluminescence under UV light. Finally, residual silver catalyst was removed from the surface by prolonged treatment (8 hours) in nitric acid.

Next, solutions of copper and lead phthalocyanines were applied to the surface of the porous silicon. $5 \cdot 10^{-4}$ M solutions of phthalocyanines in dimethyl sulfoxide (DMSO) were prepared and applied dropwise to the porous silicon surface (0.1 ml/cm²). DMSO was chosen because it is one of the few highly polar aprotic solvents capable of overcoming strong intermolecular interactions (aggregation) between phthalocyanine macrocycles and maintaining them on the surface, followed by vacuum drying at room temperature under 10^{-5} mmHg for 24 hours.

Impedance and I–V measurements. The electrophysical characteristics of the samples were measured using a modern LCR meter (ROHDE & SCHWARZ LCX 200) and the Keithley 2450 SMU system, following the methodology described in [16]. For DC I–V and impedance measurements, the contact area was formed using a thick rectangular indium (In) bar (2 mm×2 mm). The overall measurement scheme for the equivalent circuit was as follows: Bottom – Ag/In/Al/por-Si/McPc/In/Au – Top.

Processing and visualization of experimental data were performed using the OriginLab software environment. The frequency dependence of AC conductivity was studied in the |Z|–phase mode with automatic determination of all components of the complex impedance in a parallel equivalent circuit configuration.

The total conductivity (σ_{total}) consists of DC and AC components and was calculated using the formula [17]:

$$\sigma_{total}(\omega) = \sigma_{dc} + \sigma_{ac}(\omega) \quad (1)$$

For many disordered materials, including organic semiconductors, the frequency dependence of AC conductivity, $\sigma_{ac}(\omega)$, follows Jonscher's universal power law:

$$\sigma_{ac}(\omega) = A\omega^{s} \quad (2)$$

where A is a temperature-dependent pre-exponential factor, and s is a dimensionless exponent, usually in the range $0 < s < 1$.

Figure 1 shows the I–V characteristics of the investigated por-Si heterostructures in the geometry Bottom – Ag/In/Al/por-Si/McPc/In/Au – Top with copper and lead phthalocyanines, presented in linear (a) and semi-logarithmic (b) scales. From Fig. 1a, it is evident that the I–V curves are typical for a barrier structure, and the por-Si/McPc heterojunction exhibits rectifying behavior.

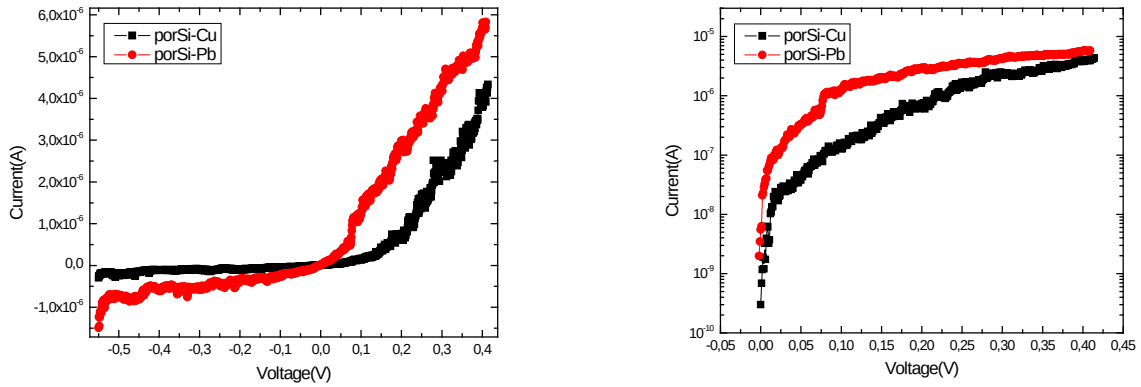
For the por-Si/CuPc structure, the forward-bias I–V curve on the semi-logarithmic plot (Fig. 1b) shows three distinct linear regions, indicating a sequential change of conduction mechanisms. The low-voltage region (I) corresponds to conduction via the thermally assisted field emission mechanism (the rectifying region). The transition to region (II) is characterized by a decrease in slope, indicating the dominance of charge carrier recombination in the space-charge region of the heterojunction. At voltages above 0.29 V, a significant downward bending of the curve occurs (region III), resulting from current limitation by the series resistance of the material.

For the por-Si/PbPc structure, the device exhibits exponential conduction only within a narrow range up to 0.006 V (linear portion of the I–V curve). At higher voltages, the curve rapidly deviates from ideal diode behavior, bending downward. This behavior indicates a much higher series resistance in the por-Si/PbPc structure, which becomes dominant even at very low currents and voltages. This may be related to the poorer intrinsic conductivity of lead phthalocyanine or to the formation of a high-resistance layer at the interface.

Fig. 2 shows the AC I–V characteristics of the investigated por-Si heterostructures in the geometry Bottom – Ag/In/Al/por-Si/McPc/In/Au – Top, presented in the Jonscher projection. For the por-Si/CuPc structure (Fig. 2a) and the por-Si/PbPc structure (Fig. 2b), the DC component in Jonscher's power law is observed up to frequencies of 10^6 rad/s, indicating the dominance of charge carrier drift over accumulation processes at interfaces or traps.

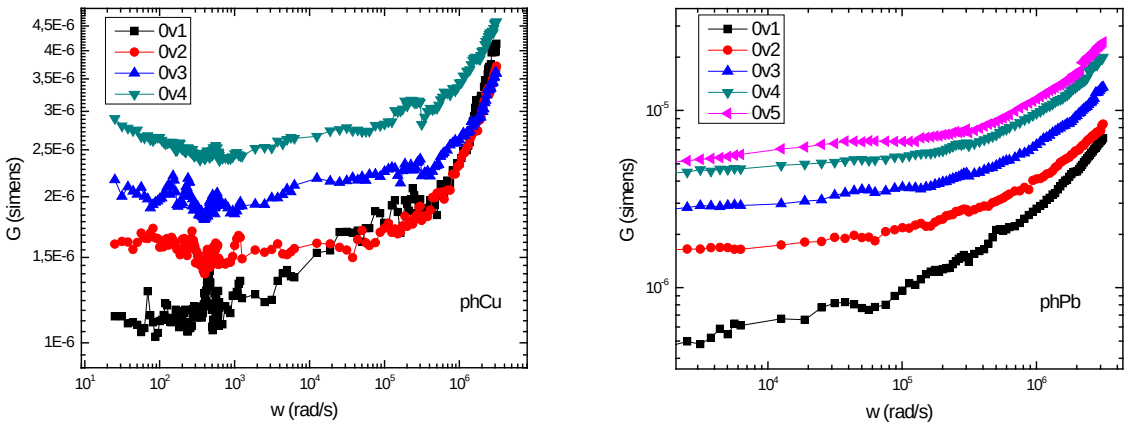
Structural modeling. The molecular structures of Cu and Pb phthalocyanines were built using Chem3D through structure optimization by minimizing the total potential energy of the molecule (MM2 minimization). The HOMO and LUMO energy levels were obtained using Chem3D's built-in Extended Hückel computational algorithm. For CuPc, the values were: LUMO = –4.02 eV; HOMO = –4.452 eV. For PbPc, the values were: LUMO = –4.526 eV; HOMO = –4.58 eV. The electronic structures of the HOMO and LUMO of CuPc, ZnPc, FePc, TiOPc, and PbPc are presented in [19], and CuPc alone was calculated using the DFT method in Gaussian09 [18].

Figure 3 shows the three-dimensional models of the copper and lead phthalocyanine macrocycles. For PbPc, before energy minimization, the Pb atom was manually placed at the center of the macrocycle to preserve planarity during the initial structural setup. However, after geometry optimization and energy minimization, the calculation algorithm displaced the Pb atom relative to the plane of the molecule.



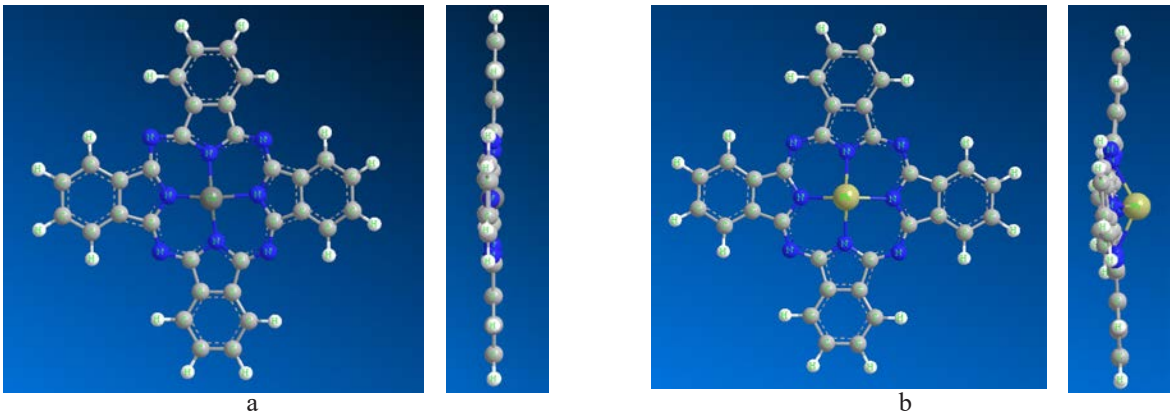
a b

Fig. 1. Current–voltage characteristics of the investigated por-Si heterostructures with copper and lead phthalocyanines in linear (a) and semi-logarithmic (b) representation



a b

Fig. 2. AC current–voltage characteristics of the investigated por-Si heterostructures with copper (a) and lead (b) phthalocyanines, presented in the Jonscher projection



a b

Fig. 3. Three-dimensional models of the copper (CuPc) and lead (PbPc) phthalocyanine macrocycles in different projections

The figure shows the resulting structures of CuPc and PbPc obtained after minimizing the total energy of each individual molecule. It is evident that the Pb atom is positioned above the plane of the macrocycle. This is due to the ionic radius of Pb^{2+} (≈119 pm) being significantly larger than that of Cu^{2+} (≈73 pm), so the lead atom cannot geometrically fit into the internal cavity of the phthalocyanine macrocycle, which consists of four indole fragments condensed into a flat aromatic heterostructure. Due to the oversized Pb^{2+} ion, the macrocycle cannot maintain planar coordination with the nitrogen atoms, resulting in pronounced non-planarity (out-of-plane displacement) for the PbPc complex.

Thus, the significantly larger size of the lead ion induces considerable strain in the molecule, increas-

ing the total energy of the complex and making the planar conformation energetically unstable. In contrast, the smaller copper ion fits perfectly into the central cavity, minimizing strain and stabilizing a planar geometry. For PbPc, displacement out of the plane and adoption of a non-planar conformation is energetically favorable. This deformation relieves internal strain and achieves a more stable configuration, despite weakening and elongating the Pb–N bonds compared to the in-plane Cu–N bonds.

The planarity of the macrocycle determines the degree of ideality of the Ag/In/Al/por-Si/McPc/In/Au heterojunction, which directly affects charge transport across the interface. A schematic representation of charge transport in a p-type organic semiconductor, based on the percolation model with variable-range hopping and multiple trapping–release mechanisms, is described in [18]. It is based on the relative positions of the LUMO and HOMO levels of the organic semiconductor with respect to the conduction and valence bands of porous silicon.

Considering that the structure uses porous silicon with crystallite sizes not exceeding 2.8 nm (to observe photoluminescence and ensure sufficient electron transport through the porous layer), the quantum confinement effect becomes dominant [20]. This significantly increases the bandgap and reduces the electron affinity to values in the range of 3.0–3.5 eV (compared to 4.05 eV for bulk Si according to tabulated data).

This critical factor alters the injection picture: the LUMO levels of both CuPc (–4.02 eV) and PbPc (–4.526 eV) are lower in energy than the reduced electron affinity of PS (3.0–3.5 eV), creating favorable conditions for electron injection from PS into the LUMO of the organic layer. Meanwhile, the HOMO levels of both macrocycles lie above the valence band of porous silicon, forming a potential barrier for hole injection.

This explains the observed non-ideal diode behavior and the early dominance of series resistance (particularly for PS/PbPc), since charge transport in forward bias is limited not by ideal Shockley diffusion but by thermal activation over these injection barriers and trap-controlled mechanisms.

Conclusions. A critical influence of the central metal on the morphology and energy alignment of the heterojunctions has been established. Modeling showed that due to the large ionic radius of Pb^{2+}, unlike Cu^{2+}, the lead phthalocyanine complex (PbPc) adopts a pronounced non-planar conformation. Analysis of the DC I–V characteristics revealed that this structural mismatch correlates with a significantly higher series resistance in the por-Si/PbPc structure, which dominates at voltages above 0.006 V, indicating the formation of a high-resistance interfacial layer and/or poorer intrinsic conductivity of the organic film compared to por-Si/CuPc.

The DC I–V analysis identified a sequential change in conduction mechanisms for CuPc and a limited diode behavior for PbPc. For the por-Si/CuPc structure, the I–V curve shows three distinct linear regions: (I) thermally assisted field emission (rectification), (II) recombination in the space-charge region (decrease in slope), and (III) current limitation by series resistance. In contrast, the rapid deviation from ideal diode behavior in por-Si/PbPc indicates early dominance of series resistance, which, combined with injection energy barriers (due to the reduced electron affinity of PS, 3.0–3.5 eV), suggests that charge transport is limited by thermal activation over barriers and/or trap-controlled mechanisms, consistent with the percolation model.

This work has been supported by the Project «Development of photovoltaic cells and thin-film photoconverters based on organic solar light absorbers» is financially supported by the Ministry of Education and Science of Ukraine, state registration number 0125U001660 and Project No. 5.8/25-П “Energy-saving and environmentally friendly nanoscale ferroics for the development of sensorics, nanoelectronics and spintronics” of the Target Program of the National Academy of Sciences of Ukraine.

Bibliography:

1. Di Sabatino M., Hendawi R., Garcia A. S. Silicon Solar Cells: Trends, Manufacturing Challenges, and AI Perspectives. *Crystals*. 2024. Vol. 14, № 2. P. 167. https://doi.org/10.3390/cryst14020167

2. Aftab S., Koyyada G., Ali Z., Assiri M. A., Kim J. H., Rubab N., Akman E. Flexible perovskite solar cells: A revolutionary approach for wearable electronics and sensors. *Materials Today Energy*. 2025. Vol. 51. P. 101872. https://doi.org/10.1016/j.mtener.2025.101872

3. Chiu K.-C., Juey L.-T., Su C.-F., Tang S.-J., Jong M.-N., Wang S.-S., Wang J.-S., Yang C.-S., Chou W.-C. Effects of source and substrate temperatures on the properties of ITO/CuPc/C60 heterostructure prepared by physical vapor deposition. *Journal of Crystal Growth*. 2008. Vol. 310. P. 1734–1738.

4. Guruswathi S., Ramesh S., Ashok Kumar A., Rajagopal Reddy V. Optical, morphological, structural and photo-electrical properties of Ni-phthalocyanine/n-Ge heterojunction for optoelectronic applications. *Thin Solid Films*. 2024. Vol. 803. P. 140460. https://doi.org/10.1016/j.tsf.2024.140460

5. Majhi J., Ghosh S., Priya K., Sharma S., Bandyopadhyay A. A critical review on the progress of emerging active and substrate materials for organic solar cells and device level fabrication techniques by solution process method. *Next Materials*. 2025. Vol. 8. P. 100595. https://doi.org/10.1016/j.nxmate.2025.100595

6. Bruder I., Schöneboom J., Dinnebier R., Ojala A., Schäfer S., Sens R., Erk P., Weis J. What determines the performance of metal phthalocyanines (MPc, M=Zn, Cu, Ni, Fe) in organic heterojunction solar cells? A combined experimental and theoretical investigation. *Organic Electronics*. 2010. Vol. 11, № 3. P. 377–387. https://doi.org/10.1016/j.orgel.2009.11.016

7. Ali I., Islam M. R., Yin J., Eichhorn S. J., Chen J., Karim N., Afroj S. Advances in Smart Photovoltaic Textiles. *ACS Nano*. 2024. Vol. 18, № 5. P. 3871–3915. https://doi.org/10.1021/acsnano.3c10033

8. Chen K.-W., Huang C.-W., Lin S.-Y., Liu Y.-H., Chatterjee T., Hung W.-Y., Liu S.-W., Wong K.-T. Merocyanines for vacuum-deposited small-molecule organic solar cells. *Organic Electronics*. 2015. Vol. 26. P. 319–326. https://doi.org/10.1016/j.orgel.2015.07.050

9. Han L.-H., Zhang C.-R., Zhe J.-W., Jin N.-Z., Shen Y.-L., Wang W., Gong J.-J., Chen Y.-H., Liu Z.-J. Understanding the Electronic Structures and Absorption Properties of Porphyrin Sensitizers YD2 and YD2-o-C8 for Dye-Sensitized Solar Cells. *International Journal of Molecular Sciences*. 2013. Vol. 14, № 10. P. 20171–20188. https://doi.org/10.3390/ijms141020171

10. Pavani M., Ashok Kumar A., Rajagopal Reddy V., Kaleemulla S., Jyothi I., Choi C.-J. Optical, morphological and electrical properties of rapid thermally annealed CoPc/n-Ge heterostructures for photodiode applications. *Materials Science and Engineering: B*. 2024. Vol. 300. P. 117102. https://doi.org/10.1016/j.mseb.2023.117102

11. Alam S., Lee J. Progress and Future Potential of All-Small-Molecule Organic Solar Cells Based on the Benzodithiophene Donor Material. *Molecules*. 2023. Vol. 28, № 7. P. 3171. https://doi.org/10.3390/molecules28073171

12. Kumar A., Vashistha V. K., Das D. K. Recent development on metal phthalocyanines based materials for energy conversion and storage applications. *Coordination Chemistry Reviews*. 2021. Vol. 431. P. 213678. https://doi.org/10.1016/j.ccr.2020.213678

13. Lai H., Li X., Li S., Chen Y., Sun B., Jiang Q., Yang J. Enhancement of photovoltaic performance and moisture stability of perovskite solar cells by modification of tin phthalocyanine (SnPc). *Electrochimica Acta*. 2019. Vol. 296. P. 799–805. https://doi.org/10.1016/j.electacta.2018.10.087

14. Nofil M., Raza E., Aziz F., Supangat A., Abbas N. Optimizing small molecule-based organic solar cells with metal phthalocyanines for enhanced efficiency and stability. *Inorganic Chemistry Communications*. 2025. Vol. 173. P. 113812. https://doi.org/10.1016/j.inoche.2024.113812

15. Arı M., Kanat Z., Dinçer H. Design, computational screening and synthesis of novel non-peripherally tetra hexylthio-substituted phthalocyanines as bulk heterojunction solar cell materials. *Solar Energy*. 2016. Vol. 134. P. 1–8. https://doi.org/10.1016/j.solener.2016.04.041

16. Mykola O. Semenenko, Sergii O. Kravchenko, Nadiia V. Siharova, Olha V. Pylypova, Mariya I. Terets, Oleksandr S. Pylypchuk, Mariia V. Voitovych, Tetiana Yu. Obukhova, Taisiia O. Kuzmenko, Andrey Sarikov Dispersed multi-walled carbon nanotubes in polyvinyl butyral matrix for transparent ionic conductive films https://doi.org/10.48550/arXiv.2509.07584

17. Priscilla P et al Effect of carbon dots on tuning molecular alignment, dielectric and electrical properties of a smectogenic cyanobiphenyl-based liquid crystal material 2024 J. Phys. D: Appl. Phys. 57 355302 DOI 10.1088/1361-6463/ad4a84

18. Rani V. et al. Charge transport mechanism in copper phthalocyanine thin films with and without traps. RSC Advances. 2017. Vol. 7, Iss. 86. P. 54911–54917. doi:10.1039/c7ra08316e.

19. Baba S., Suzuki A., Oku T. Electronic structures and magnetic/optical properties of metal phthalocyanine complexes. AIP Conference Proceedings. 2016. Vol. 1709. 020012. doi: 10.1063/1.4941211.

20. Semenenko et. all. J. Appl. Phys. 128, 114302 (2020); doi: 10.1063/5.0020527

Семененко М.О., Обухова Т.Ю., Коваль В.М., Кравченко С.О., Чопик В.В., Саріков А.В.

ЕЛЕКТРОФІЗИЧНІ ВЛАСТИВОСТІ ГЕТЕРОСТРУКТУР З ШАРАМИ ФТАЛОЦІАНІНІВ ДЛЯ ФОТОВАЛЬТОЇЧНОГО ЗАСТОСУВАННЯ

У статті досліджено електрофізичні властивості гетероструктур на основі пористого кремнію з нанесеними шарами фталоціанінів міді та свинцю, що є перспективними органічними матеріалами для фотовольтаїки нового покоління. Актуальність дослідження зумовлена пошуком недорогих, гнучких та стабільних органічних фотоперетворювачів, здатних доповнити або замінити традиційні кремнієві сонячні елементи. Отримання пористого шару здійснювали методом метал-стимульованого травлення, після чого на підготовлену поверхню наносили розчини CuPc та PbPc у ДМСО. Електрофізичні характеристики досліджували за допомогою імпедансної спектроскопії та

вимірювання DC ВАХ. Показано, що гетероструктури демонструють випрямляючу поведінку, проте механізми провідності істотно залежать від виду центрального металу у макроциклі. Для структури por-Si/CuPc виявлено три характерні області провідності, що відповідають термічно-польовій емісії, рекомбінаційним процесам у області просторового заряду та лімітації струму послідовним опором. У випадку por-Si/PbPc встановлено домінування послідовного опору вже за наднизьких напруг (понад 0.006 В), що свідчить про формування високоомного інтерфейсу та гірші транспортні властивості порівняно з CuPc. Наведене в статті молекулярне моделювання CuPc і PbPc показало, що комплекс свинцю є суттєво непланарним через значно більший іонний радіус Pb^{2+}, тоді як CuPc зберігає плоску конформацію. Непланарність PbPc зумовлює збільшення внутрішньої напруги в молекулі та погіршення енергетичного вирівнювання на гетеропереході, що корелює зі спостереженою високою величиною послідовного опору. Аналіз частотної залежності провідності підтвердив домінування дрейфового механізму транспорту заряду до частот 10^6 рад/с для обох структур. Отримані в статті результати демонструють критичну роль центрального металу у формуванні енергетичних бар'єрів і транспортних властивостей гетероструктур por-Si/McPc та визначають CuPc як більш придатний матеріал для створення ефективних органічно-неорганічних фотоперетворювачів.

Ключові слова: *плівки метал-фталоцианінів, макроцикл, органічний гетероперехід, пористий кремній, вольт-амперні характеристики.*

Дата надходження статті: 25.11.2025
Дата прийняття статті: 11.12.2025
Опубліковано: 30.12.2025