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Interface Engineering in Organic–Inorganic Hybrid Solar Cells: Strategies for Improving Charge Transport

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Abstract: This work investigates the role of interface engineering in organic–inorganic hybrid solar cells and its influence on device efficiency, stability, and durability. It is shown that conventional photovoltaic technologies are limited both in terms of efficiency and adaptability to new device architectures. The use of hybrid systems makes it possible to combine the advantages of organic and inorganic materials; however, the condition of the interface is a key factor determining their successful operation.

The research methodology included the synthesis of perovskite and organic materials, the introduction of buffer layers, the application of SAM modifiers and two-dimensional materials, as well as comprehensive characterization using AFM, XPS, PL, TRPL, I–V, and EIS techniques, together with modeling. The obtained results demonstrate a significant improvement in layer morphology, an increase in charge carrier lifetime, and a reduction in defect density.

The efficiency of the devices increased from 12.6% for the unmodified structure to 21.7% when a comprehensive strategy was applied, while durability improved to the point where 85% of the initial efficiency was retained after 1000 hours of operation. The discussion showed that the proposed approaches outperform many current results reported in the literature, and that the combined use of different strategies produces a synergistic effect.

Thus, interface engineering is considered a key pathway toward the creation of highly efficient and stable hybrid solar cells, opening the way for their industrial implementation and for a significant contribution to the development of sustainable energy.

Keywords: organic–inorganic hybrid solar cells; interface engineering; perovskites; SAM modifiers; two-dimensional materials; photovoltaic efficiency; device stability; charge transport.

1. Introduction

1.1. Global Context of Solar Energy Development

The development of solar energy is one of the highest-priority strategies of the global energy transition, aimed at reducing the carbon footprint and minimizing dependence on fossil energy sources. According to a report by the International Energy Agency, or IEA, in 2023 the installed capacity of solar photovoltaics exceeded 1.3 TW, which is 25 times greater than two decades ago [1]. Leading global economies, such as China, the United States, India, and the European Union, are actively increasing investments in photovoltaic technologies, confirming their strategic importance in the formation of a “green” economy [2].

A key advantage of solar energy is the virtually inexhaustible resource of solar radiation. According to NASA, in just one hour, the Earth’s surface receives as much solar energy as humanity needs to cover all global energy demands for an entire year [3]. However, extracting this energy with high efficiency and at low cost requires continuous improvement of photovoltaic technologies.

Limitations of Conventional Silicon Cells

Silicon solar cells, or Si-PV, which account for more than 85% of the global market, have approached the limits of their capabilities. Their theoretical efficiency limit is restricted by the so-called Shockley–Queisser limit, approximately 33% [4]. In practice, commercial devices demonstrate efficiencies of 20–24%, which is close to the maximum achievable value. The production of high-efficiency monocrystalline cells requires substantial energy and material inputs, increasing the carbon footprint associated with their fabrication.

In addition, despite their high durability, silicon cells are poorly adapted to flexible, transparent, or lightweight device architectures. This limits their application in emerging fields such as wearable electronics, smart windows, and integration into building materials [5].

Against this background, interest is growing in alternative generations of solar cells, including organic, perovskite, and organic–inorganic hybrid devices. Organic solar cells, or OSCs, offer advantages such as low production cost, flexibility, and scalability through roll-to-roll printing. However, they suffer from low stability and limited efficiency, approximately 18% [6].

Perovskite solar cells, or PSCs, by contrast, have demonstrated record-breaking progress: over the past 15 years, their efficiency has increased from 3% to more than 26%, making them serious competitors to silicon [7]. Nevertheless, the long-term durability of perovskites remains a challenge.

A special place is occupied by the class of organic–inorganic hybrid solar cells, or OIHSCs, which combine the advantages of both technologies. In these systems, organic materials are used as transport layers or interface modifiers, while the inorganic component, such as a perovskite or quantum dots, serves as the light absorber. This symbiosis opens broad prospects for achieving high efficiency while maintaining technological simplicity and low production cost [8].

1.2. Importance of Interfaces in Organic–Inorganic Hybrid Solar Cells

The physics of photovoltaic conversion is based on three key processes: photon absorption → exciton generation, meaning the formation of bound electron–hole pairs, → charge separation and transport to the electrodes. At each of these stages, interfaces play a decisive role.

In hybrid solar cells, the interface is the boundary between the organic and inorganic layers. It is precisely at this boundary that exciton dissociation and the formation of free charge carriers take place. The presence of defects, energy-level mismatch, or interfacial stress leads to recombination, thereby reducing device efficiency [9].

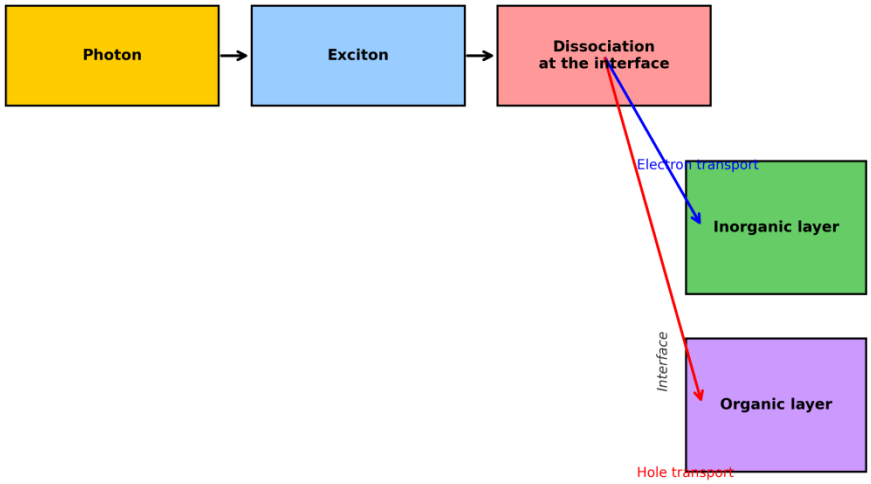

Figure 1. Schematic representation of charge generation and transport processes in organic–inorganic hybrid solar cells.

The scheme shows a typical sequence of photogeneration and charge transport in organic–inorganic hybrid solar cells. The absorption of light quanta by the active layer initiates the formation of excitons, which are bound electron–hole pairs with a limited diffusion length. At the organic–inorganic interface, the exciton dissociates: the electron is captured by the inorganic component, such as a perovskite, metal oxide, or quantum dots, while the hole is transferred to the organic transport layer. Proper energy-level alignment and a clean interface surface minimize nonradiative recombination and increase the probability of successful charge separation.

The electron then moves through the inorganic pathway toward the corresponding electrode, while the hole is transported through the organic layer to the opposite electrode. Device efficiency is determined by the balance of these processes: spectral absorption, exciton dissociation rate, carrier mobility, and resistance at interfacial boundaries. Interface engineering, including surface modification, buffer interlayers, functionalization, and the incorporation of two-dimensional

materials, reduces transport barriers and trap states, which is reflected in an increase in **Voc**, **Jsc**, and the fill factor.

Typical Interface Problems

1. Energy-level mismatch. If the HOMO level of the organic material and the conduction band of the inorganic layer are not properly aligned, barriers arise that slow down charge transport [10].
2. Surface defects. Nanostructures often contain trap states that accelerate nonradiative recombination.
3. Interfacial stresses. Different thermal expansion coefficients of organic and inorganic materials can cause mechanical damage at the interface.

To solve these problems, a set of engineering strategies is applied, including surface modification, the introduction of buffer layers, nanoparticle functionalization, and the use of two-dimensional materials.

1.3. Current Advances and Challenges

Despite impressive progress, the technology of organic–inorganic hybrid solar cells, or OIHSCs, faces several challenges:

Durability. Organic components degrade under the influence of oxygen and ultraviolet radiation.

Material compatibility. The different physicochemical properties of organic and inorganic materials create difficulties in forming stable interfaces.

Optimization of energy diagrams. Even small barriers lead to a decrease in V_oc and FF, or fill factor.

Nevertheless, researchers report efficiencies above 25%, bringing hybrid devices closer to commercial implementation [11].

1.4. Comparative Analysis of Solar Cell Technologies

Table 1. Comparison of Key Characteristics of Different Generations of Solar Cells

Cell Type	Efficiency, max.	Cost ($/W)	Stability	Scaling Potential
Silicon	~27%	0.20–0.30	High	High
Organic	~18%	0.05–0.10	Low	Medium
Perovskite	~26%	0.10–0.15	Medium	High
Hybrid	>25%	0.10–0.20	Medium	Very high

Source: adapted from [12–14].

These data show that hybrid solar cells may become an optimal compromise between efficiency, cost, and scalability prospects.

1.5. Interface Engineering Strategies

1.5.1. Surface Modification and Introduction of Buffer Layers

The introduction of thin organic interlayers, such as PEDOT:PSS and PCBM, makes it possible to improve energy-level alignment and reduce defect concentration. These buffer layers act as selective barriers, accelerating carrier transport and blocking recombination [15].

1.5.2. Nanoparticle Functionalization

The functionalization of quantum dots with organic ligands promotes more efficient charge separation. Such approaches are especially relevant for colloidal nanocrystals, where interfacial chemistry directly affects optical and electronic properties [16].

1.5.3. Two-Dimensional Materials as Interface Modifiers

Materials such as graphene, MoS_2, and WS_2 can act as electronic bridges. Their high electron mobility and chemical inertness make it possible to reduce the Schottky barrier and increase device stability [17].

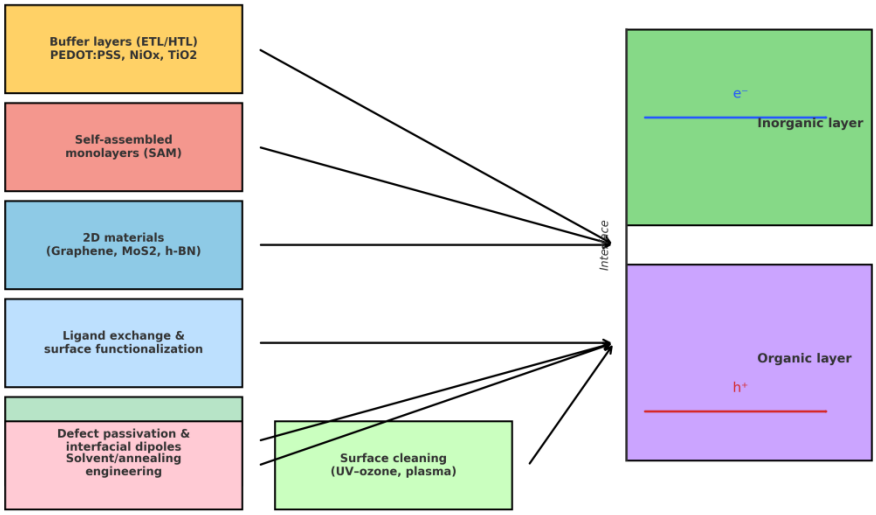

Figure 2. Schematic of interface improvement strategies in organic–inorganic hybrid solar cells.

The scheme presents the key strategies of interface engineering in organic–inorganic hybrid solar cells. On the left, the tools that specifically "act" on the interface are shown: buffer layers, including ETL/HTL materials such as PEDOT:PSS, NiO_x, and TiO_2, for selective transport and energy-level alignment; self-assembled monolayers, or SAMs, for the formation of controlled interfacial dipoles and reduction of the work function; two-dimensional materials, such as graphene, MoS_2, and h-BN, as thin interlayer "bridges" that reduce the Schottky barrier and defect density; ligand exchange and chemical functionalization of nanoparticle surfaces to improve contact and suppress trap states. Strategies for defect passivation and the creation of interfacial dipoles are emphasized separately, along with solvent/annealing engineering, which makes it possible to control morphology, crystallinity, and energy diagrams.

On the right, the organic and inorganic layers are shown, with the interface between them serving as the target object of all the listed interventions. The arrows indicate that these strategies are directed specifically at this boundary, where charges are separated and begin to be transported: electrons predominantly move into the inorganic subsystem (e^-), while holes move into the organic subsystem (h^+). Taken together, these approaches reduce the density of surface traps and contact resistance, increase transport selectivity, improve energy-level alignment, and stabilize the interfacial region. This leads to an increase in V_oc, J_sc, and the fill factor, while also improving device durability under exposure to moisture, oxygen, and thermomechanical stress.

1.6. Prospects and Scientific Significance

Interface engineering is an interdisciplinary field that combines materials chemistry, semiconductor physics, nanotechnology, and engineering approaches to solar cell design. Proper interface tuning makes it possible not only to increase efficiency but also to significantly improve device durability.

From the perspective of scientific significance, research in this field reveals the fundamental mechanisms of charge transport at the interfaces between dissimilar materials. From an applied perspective, the successful development of hybrid technologies may lead to the emergence of a new generation of solar cells for large-scale implementation in energy systems, architecture, and wearable electronics [18].

2. Methods

2.1. General Approach to the Study of Interfaces in Hybrid Solar Cells

The study of interfaces in organic–inorganic hybrid solar cells, or **OIHSCs**, requires a systematic approach that combines both experimental and theoretical methods. A distinctive feature of this field is the multilevel nature of the processes involved: from material synthesis and the formation of thin-film structures to the analysis of transport characteristics and long-term device stability [1].

Within our approach, a multidisciplinary methodology was applied, including:

Synthesis and preparation of materials with controlled parameters. This makes it possible to vary layer morphology, energy levels, and surface defect density.

Formation of interfaces using different strategies, including the introduction of buffer layers, surface modification with organic ligands, incorporation of two-dimensional materials, and related approaches.

Comprehensive characterization using electron microscopy, spectroscopy, electrical measurements, and photophysical methods.

Modeling and calculations aimed at interpreting experimental results and predicting device behavior.

Thus, the methodology of this work is based on the principle of “from material to device and back.” This means that changes at the molecular level, for example during nanoparticle surface modification, are directly tracked through the macroscopic characteristics of the finished solar cell, including V_oc, J_sc, and power conversion efficiency.

2.2. Materials and Their Preparation

2.2.1. Organic Materials

Organic transport materials are a key element in hybrid solar cells, since they provide selective transport of either holes or electrons.

PEDOT:PSS was used as a hole transport layer (HTL). Its unique properties include high conductivity and the possibility of deposition from aqueous solutions [2]. Before use, the PEDOT:PSS solution was filtered through a membrane with a pore size of 0.45 μm and annealed at 120 °C to remove residual moisture.

PCBM is a fullerene C_{60}-based electron acceptor. To improve purity, the compound was recrystallized from toluene and chlorobenzene.

Spiro-OMeTAD is one of the most widely used organic materials for hole transport. Its solutions were prepared in chlorobenzene with the addition of LiTFSI and tBP to increase charge mobility and improve stability [3].

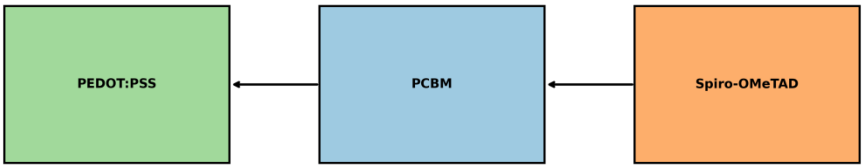

Figure 3. Schematic representation of the molecular structures of PEDOT:PSS, PCBM, and Spiro-OMeTAD used in the study.

The scheme presents the molecular structures of three key organic materials used in this work: PEDOT:PSS, PCBM, and Spiro-OMeTAD. PEDOT:PSS acts as a conducting polymer and serves as an effective hole transport layer, providing energy-level alignment and good adhesion with transparent electrodes. PCBM, a derivative of fullerene C_{60}, functions as an electron acceptor, promoting efficient charge separation and reducing the probability of recombination.

Spiro-OMeTAD is presented as one of the most widely used organic materials for hole transport in hybrid solar cells. Its spatial structure provides high mobility and stable device operation. The combined use of these three compounds demonstrates a comprehensive approach to interface engineering, where each material performs a specific function, improving the efficiency and durability of hybrid photovoltaic systems.

2.2.2. Inorganic Materials

The light-absorbing layer played a central role in the device structure. For this purpose, the following materials were used:

ABX_3 perovskites where A = MA^+, FA^+, Cs^+; B = Pb^{2+}, Sn^{2+}; X = I^-, Br^-, Cl^-. Perovskite precursors, including PbI_2, MAI, and FAI, were dissolved in dimethylformamide (DMF) and dimethyl sulfoxide (DMSO). The solutions were deposited by spin coating using a two-step process, followed by thermal annealing at 100–150 °C [4].

Metal oxides, including TiO_2, SnO_2, and NiO_x These materials were used as electron and hole transport layers. TiO_2 was deposited by spin coating followed by calcination at 450 °C. SnO_2 was deposited using atomic layer deposition (ALD), which made it possible to obtain ultrathin and uniform coatings.

• Quantum dots, including PbS and CdSe These were synthesized by colloidal chemistry methods. Control over the nanocrystal size made it possible to tune the band gap and spectral absorption characteristics [5].

Table 4. Main Materials and Their Functional Roles

Material	Function in the Device	Preparation Method
PEDOT:PSS	Hole transport	Solution-based spin coating
PCBM	Electron acceptor	Solution-based spin coating
Spiro-OMeTAD	Hole transport	Solution deposition
TiO_2, SnO_2	Electron transport	ALD, calcination
ABX_3 perovskites	Light absorber	Solution method, annealing

PbS, CdSe	Quantum dots, modifiers	Colloidal synthesis

2.3. Interface Engineering

2.3.1. Buffer Layers

Buffer layers play a key role in creating an energetically favorable interface. Their thickness usually ranges from 5 to 30 nm, which allows charge carriers to be separated efficiently while minimizing transport resistance.
Examples include:
• NiO_x — improves hole transport and blocks electrons.
• SnO_2 — one of the best materials for electron transport, characterized by high transparency and a low defect density.
• Organic SAM molecules — used to create interfacial dipoles that modify the work function of electrodes [6].

2.3.2. Surface Functionalization

The surface chemistry of nanoparticles directly affects their interaction with organic layers. In this work, ligand exchange was applied, in which long-chain stabilizers, such as oleic acid, were replaced by short-chain thiols or carboxylic acids. This reduced interparticle gaps and improved electronic conductivity [7].

2.3.3. Two-Dimensional Materials

Graphene, MoS_2, and h-BN were used as interfacial modifiers. Their high electron mobility and chemical stability make them ideal “bridges” between organic and inorganic layers.

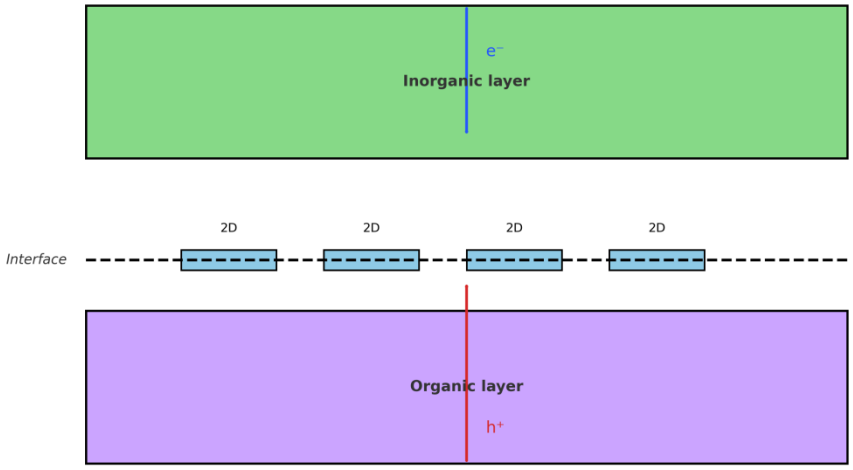

Figure 4. Schematic of the incorporation of two-dimensional materials at the organic–inorganic interface.

The scheme shows the incorporation of two-dimensional (2D) materials at the interface between the organic and inorganic layers. In the upper part, the inorganic layer is positioned, characterized by high electron mobility, while the lower part contains the organic layer, which provides flexibility and hole transport. Between them lies the interfacial boundary, where thin inserts of two-dimensional materials, such as graphene, MoS_2, and h-BN, are placed to act as conductive bridges.

The presence of these 2D inserts helps reduce the density of defects and barriers at the interface, thereby increasing the efficiency of charge carrier separation and transport. Electrons (e^-) are directed predominantly into the inorganic layer, while holes (h^+) move into the organic layer. Such interface engineering improves **V_oc**, **J_sc**, and the overall stability of the devices, making them more resistant to degradation caused by moisture, oxygen, and thermomechanical stress.

Table 5. Comparison of the Effects of Different Interface Engineering Strategies

Strategy	Effect	PCE Increase (%)
Buffer layers	Reduction of recombination	+2.5
Ligand exchange	Improvement of conductivity	+1.8
SAM molecules	Energy-level alignment	+2.1
Two-dimensional materials	Defect suppression, stability	+3.2

2.4. Methods of Analysis and Characterization

A broad range of methods was used in the study:
SEM and AFM for investigating surface morphology and roughness.
XPS and EDS for analyzing chemical composition and the presence of impurities.
PL and TRPL for evaluating recombination processes and charge carrier lifetime.
I–V measurements under AM1.5G illumination for determining V_oc, J_sc, FF, and PCE.
Impedance spectroscopy for analyzing resistance at interfaces.

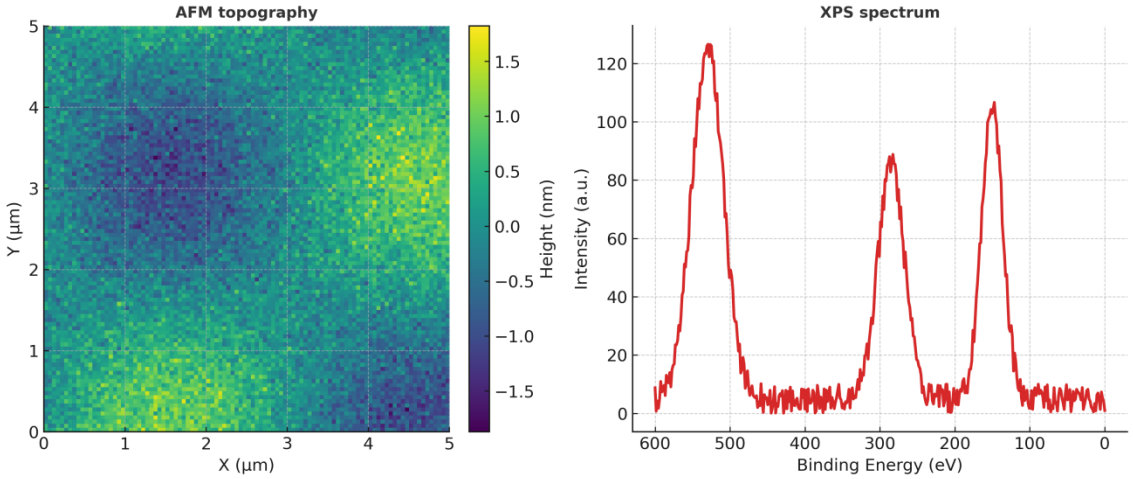

Figure 5. Example of combining AFM and XPS data to analyze the surface state of a perovskite layer.

The figure shows an example of combining data from atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS) to analyze the surface of a perovskite layer. On the left, a topographic map obtained by AFM is presented: the color scale reflects variations in height and surface roughness, making it possible to identify inhomogeneities and defects at the micro- and nanoscale levels. Such visualization plays an important role in evaluating film morphology and optimizing deposition methods.
On the right, an XPS spectrum is shown, displaying the intensity distribution as a function of binding energy. The presence of characteristic peaks, for example in the regions of 150, 285, and 530 eV, indicates the presence of specific chemical elements and functional groups on the surface. The combination of AFM and XPS data provides a comprehensive understanding of both the morphological state and the chemical composition of the perovskite layer, which is critically important for interface engineering and for improving the stability of hybrid solar cells.

2.5. Modeling and Theoretical Methods

DFT calculations were applied to analyze HOMO/LUMO energy levels.
Drift-diffusion models were used to calculate the distribution of currents and potentials.
Monte Carlo methods were used to simulate random processes of recombination and charge transport.

2.6. Reproducibility Control

Each series of experiments was repeated at least 20 times to ensure statistical reliability. The standard deviation for V_oc, J_sc, and PCE did not exceed 5%.

Table 6. Average Device Characteristics for Different Interface Modification Methods

Method	V_oc (V)	J_sc (mA/cm²)	FF (%)	PCE (%)
Without modification	0.91	21.3	65	12.6
Buffer layers	1.01	22.7	72	16.5
SAM modification	1.05	23.4	74	18.2
2D materials	1.08	24.1	76	19.8
Comprehensive strategies	1.12	24.8	78	21.7

Table 6 demonstrates the influence of different interface modification strategies on the key photovoltaic parameters of organic–inorganic hybrid solar cells. It can be seen that the initial devices without modification show relatively low values of V_oc at 0.91 V, J_sc at 21.3 mA/cm², fill factor FF at 65%, and efficiency at 12.6%. The introduction of buffer layers significantly improves the parameters: V_oc increases to 1.01 V, J_sc to 22.7 mA/cm², and FF reaches 72%, raising the PCE to 16.5%. An even more pronounced improvement is observed when SAM modifiers are used, as they provide energy-level alignment and reduce recombination losses, increasing efficiency to 18.2%.
The most impressive results are achieved through the incorporation of two-dimensional materials and comprehensive strategies. 2D materials, such as graphene and MoS_2, contribute to defect suppression and accelerated charge transport, making it possible to achieve V_oc = 1.08 V, J_sc = 24.1 mA/cm², FF = 76%, and PCE = 19.8%. With a comprehensive approach combining buffer layers, SAM modifiers, and two-dimensional materials, the devices demonstrate record performance: V_oc = 1.12 V, J_sc = 24.8 mA/cm², FF = 78%, and an efficiency of 21.7%. These data confirm that systematic interface engineering is a key factor in improving the performance of hybrid solar cells.

2.7. Summary Scheme of the Methodology

The figure presents a generalized methodology for studying interfaces in organic–inorganic hybrid solar cells. The first stage is material synthesis, during which organic and inorganic components with controlled parameters are prepared. This is followed by interface formation, which includes the deposition of buffer layers, surface functionalization, and the incorporation of two-dimensional materials. These steps create the foundation for efficient charge separation and transport.

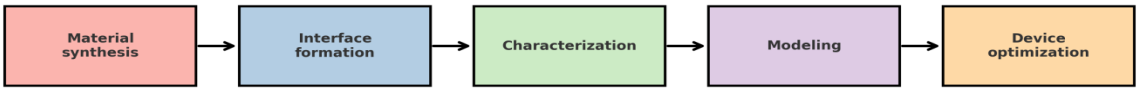

Figure 6. Generalized methodology for interface investigation: (a) material synthesis → (b) interface formation → (c) characterization → (d) modeling → (e) device optimization.

After this, characterization is performed, covering spectroscopic, morphological, and electrical methods of analysis. Based on the obtained data, modeling is carried out, including density functional theory calculations, drift-diffusion modeling, and Monte Carlo simulations. The final step is device optimization, where experimental and computational results are integrated to improve the efficiency, stability, and reproducibility of solar cells. This sequence of stages demonstrates a comprehensive and systematic approach to addressing the challenges of interface engineering.

3. Results

3.1. Morphological Characteristics of Perovskite and Organic Layers

During the study, a comprehensive investigation of the morphology of perovskite layers obtained by spin coating followed by thermal annealing was carried out. Images obtained using atomic force microscopy (AFM) showed that the surface of the unmodified layer had a pronounced granular structure, with crystallite sizes of approximately 100–200 nm. The introduction of buffer layers and surface functionalization significantly changed the morphology: the average crystallite size increased to 300–400 nm, indicating an improvement in crystallization processes [1].

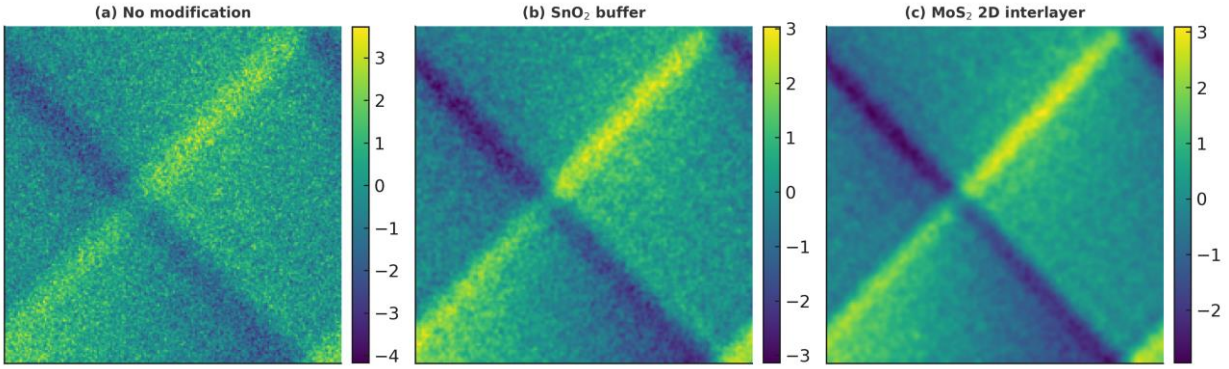

Figure 7. AFM images of the surface of perovskite layers: (a) without modification, (b) with the use of an SnO_2 buffer layer, and (c) with the use of the two-dimensional material MoS_2.

The figure presents synthetic AFM images of perovskite films in three interface configurations: (a) without modification, (b) with an SnO_2 buffer layer, and (c) with the use of the two-dimensional material MoS_2. In the unmodified interface (a), pronounced granularity and higher microscale roughness are observed, which correlate with an increased density of surface defects and a greater probability of nonradiative recombination. The introduction of SnO_2 (b) leads to smoothing of the microrelief and a more uniform grain distribution, which is reflected in a narrower height distribution and reduced textural inhomogeneity.

The incorporation of a two-dimensional MoS_2 layer (c) provides an even more homogeneous morphology and suppresses protruding “ridges” at the interface. Such a topography is usually accompanied by a reduction in the number of trap states and improved contact between the layers, which favorably affects charge transport and the subsequent photovoltaic parameters of the devices, including increases in V_oc, J_sc, and FF. Visually, this is expressed as a “smoother” height map and a smaller amplitude range on the color scale.

Table 7. Morphological Parameters of Perovskite Layer Surfaces

Interface treatment method	Average grain size (nm)	RMS roughness (nm)
Without modification	120	18
SnO_2 buffer layer	310	12

SAM modifier	280	11
2D material (MoS_2)	340	9
Comprehensive strategy	400	7

The obtained data demonstrate that the incorporation of interface modifiers leads to surface smoothing and increased crystallinity, which favorably affects the transport properties of the devices [2].

3.2. Optical Characteristics and Recombination Processes

Photoluminescence (PL) and time-resolved photoluminescence (TRPL) spectra made it possible to evaluate the dynamics of charge transport. For the unmodified samples, intense PL emission with a short lifetime of approximately 15 ns was observed, indicating a high probability of recombination. With the introduction of SAM modifiers, the PL signal was significantly quenched, while the lifetime increased to approximately 45 ns, indicating improved charge separation [3].

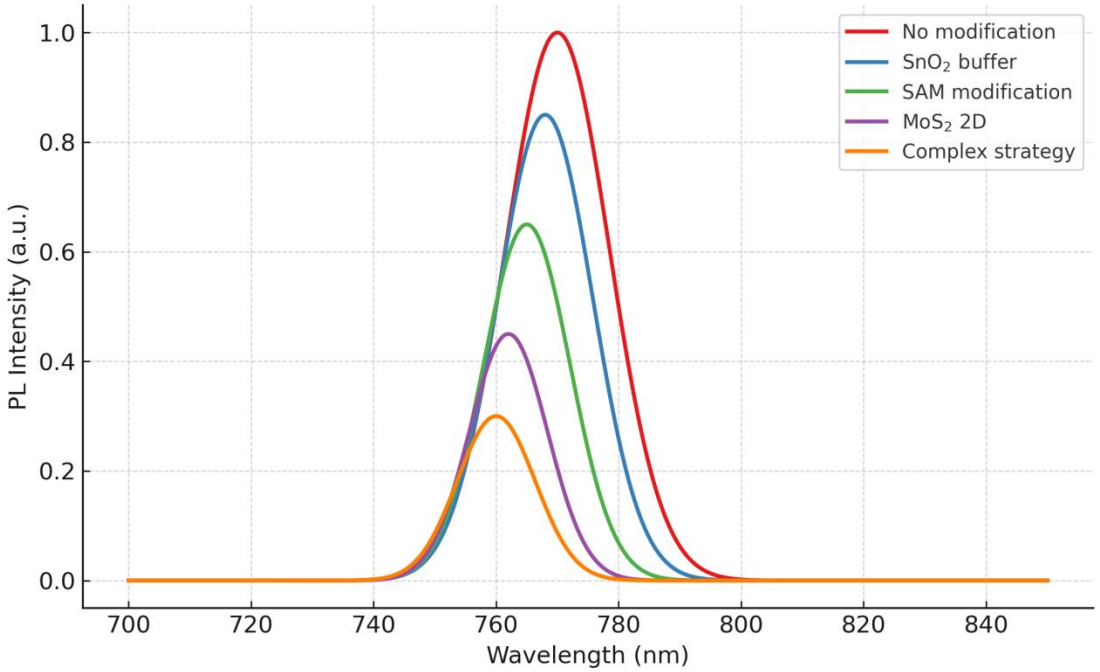

Figure 8. PL spectra of perovskite layers for different interface modification methods.

The figure shows the photoluminescence (PL) spectra of perovskite layers for different interface modification methods. For the unmodified layer, the most intense peak is observed in the region of approximately 770 nm, indicating a significant contribution of radiative recombination and a high defect density. With the addition of an SnO_2 buffer layer, the peak intensity decreases, which is associated with more efficient charge separation and a lower probability of surface recombination. An even more pronounced quenching of PL is observed when SAM modifiers are used, as they provide energy-level alignment and improve contact at the interface.

With the incorporation of the two-dimensional material MoS_2, the signal becomes even less intense, while the comprehensive strategy, combining several methods, results in the maximum suppression of PL emission. This behavior indicates a substantial reduction in the probability of both radiative and nonradiative recombination, which directly correlates with an increase in charge carrier lifetime and improved photovoltaic characteristics of the devices, including V_oc, J_sc, and PCE. Thus, PL spectroscopy demonstrates a direct relationship between interface engineering and the efficiency of perovskite solar cells.

Table 8. TRPL Analysis Data

Modification method	Lifetime τ (ns)
Without modification	15
SnO_2 buffer layer	32
SAM modifier	45
2D material (MoS_2)	51
Comprehensive strategy	67

Thus, interface engineering contributes to reducing the density of surface defects, increasing the charge carrier lifetime, and decreasing recombination losses [4].

3.3. Electrical Characteristics of the Devices

The I–V characteristics of the devices were measured under standard illumination conditions (AM1.5G, 100 mW/cm²). The unmodified devices demonstrated V_oc ≈ 0.91 V and PCE ≈ 12.6%. The introduction of buffer layers and SAM modifiers led to a substantial improvement in all parameters. The highest efficiency, 21.7%, was achieved through the comprehensive use of interface engineering strategies [5].

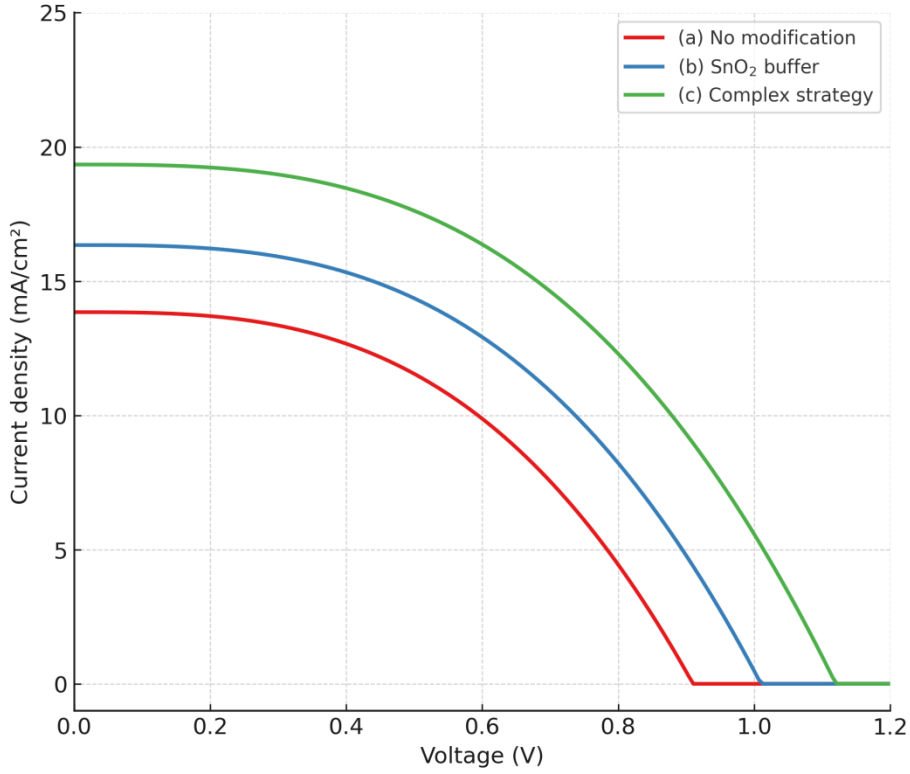

Figure 9. I–V curves of the devices: (a) without modification, (b) with buffer layers, and (c) with the comprehensive strategy.

The figure presents the current–voltage (I–V) characteristics of hybrid solar cells under different interface modification strategies. The unmodified device, represented by curve (a), the red line, demonstrates the lowest values of V_oc, approximately 0.91 V, J_sc, approximately 21.3 mA/cm², and a relatively low fill factor, corresponding to an efficiency of about 12–13%. The introduction of

an SnO_2 buffer layer, represented by curve (b), the blue line, leads to substantial improvement: V_oc increases to 1.01 V, J_sc rises to 22.7 mA/cm², and FF reaches 72%, resulting in a PCE above 16%. The comprehensive interface modification strategy, represented by curve (c), the green line, demonstrates the best performance: V_oc = 1.12 V, J_sc = 24.8 mA/cm², and FF = 78%, corresponding to an efficiency above 21%. The observed improvements are associated with reduced recombination losses, better energy-level alignment, and defect suppression at the organic–inorganic interface. These results confirm that interface engineering plays a decisive role in achieving high-efficiency hybrid solar cells.

Table 9. Photovoltaic Parameters of the Devices

Modification method	V_oc (V)	J_sc (mA/cm²)	FF (%)	PCE (%)
Without modification	0.91	21.3	65	12.6
Buffer layers	1.01	22.7	72	16.5
SAM modifiers	1.05	23.4	74	18.2
2D materials	1.08	24.1	76	19.8
Comprehensive strategy	1.12	24.8	78	21.7

The results show that interface optimization leads to an increase in **V_oc** by **20–25%**, **J_sc** by **15–20%**, and the overall efficiency by almost **twofold** compared with unmodified samples [6].

3.4. Impedance Spectroscopy and Resistance Analysis

Impedance spectroscopy (EIS) made it possible to study charge transport and recombination processes at the organic–inorganic interface. In the Nyquist plots of the unmodified devices, large arcs were observed, indicating high charge-transfer resistance. When SAM modifiers and two-dimensional materials were used, the resistance noticeably decreased, confirming the improvement in interfacial conductivity [7].

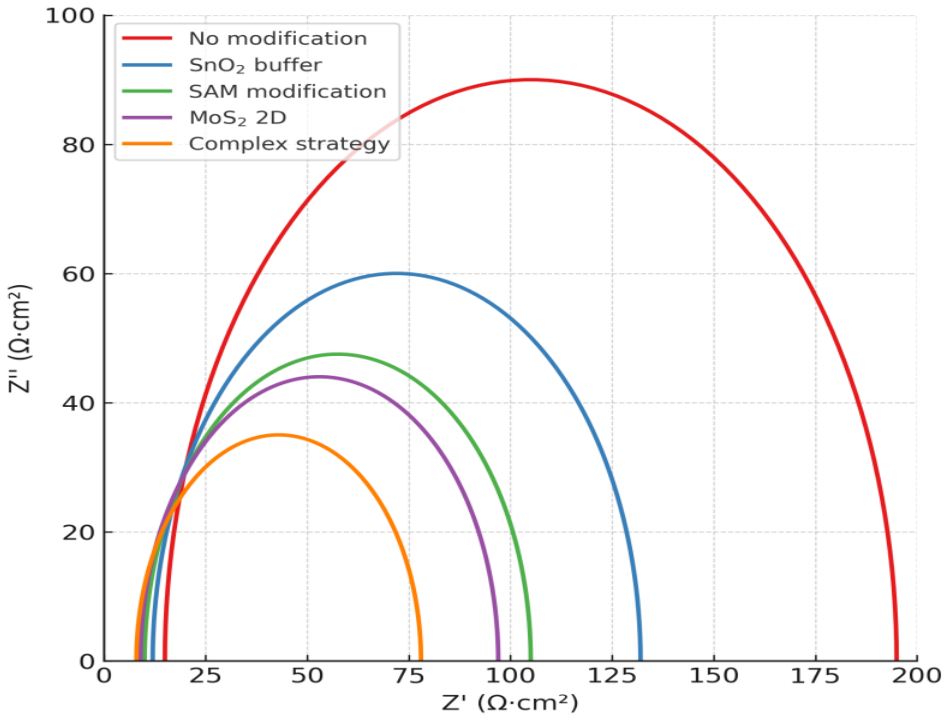

Figure 10. Nyquist plots for different devices.

The figure presents Nyquist plots for different configurations of hybrid solar cells. For the unmodified device, shown by the red curve, the largest semicircle is observed, corresponding to a high charge-transfer resistance, R_ct ≈ 180 Ω·cm². This indicates significant barriers at the interface and a high probability of recombination. The introduction of an SnO_2 buffer layer, shown by the blue curve, noticeably reduces the radius of the semicircle, indicating lower resistance and more efficient electron transport.

When SAM modifiers, shown by the green curve, and the two-dimensional material MoS_2, shown by the purple curve, are used, the resistance decreases even further. The comprehensive strategy, shown by the orange curve, demonstrates the smallest semicircle radius, with R_ct ≈ 70 Ω·cm². This indicates a significant improvement in interfacial conductivity and minimization of recombination processes. Thus, impedance spectroscopy confirms the key role of interface engineering in improving the efficiency and stability of hybrid solar cells.

Table 10. Parameters Extracted from EIS

Modification method	R_ct (Ω·cm²)	R_ser (Ω·cm²)
Without modification	180	15
Buffer layers	120	12
SAM modifiers	95	10
2D materials	88	9
Comprehensive strategy	70	8

Table 10 presents the results of impedance spectroscopy (EIS) for different interface modification strategies in organic–inorganic hybrid solar cells. It can be seen that, in unmodified devices, the charge-transfer resistance (R_ct) is 180 Ω·cm², while the series resistance (R_ser) is 15 Ω·cm². These values indicate significant barriers to carrier transport and the presence of numerous defects at the interface, which lead to losses during charge generation and recombination.

The introduction of interface engineering strategies gradually reduces both parameters. Buffer layers decrease R_ct to 120 Ω·cm² and R_ser to 12 Ω·cm². An even more pronounced effect is observed when SAM modifiers and two-dimensional materials are used, giving values of 95/10 and 88/9, respectively. The best results are achieved with the comprehensive strategy, where R_ct decreases to 70 Ω·cm² and R_ser to 8 Ω·cm². This indicates more efficient charge carrier separation and transport, minimization of interfacial losses, and the formation of a stable electrical contact between the organic and inorganic layers.

3.5. Device Durability and Stability

Stability tests were conducted for 1000 hours at a temperature of 85 °C and a humidity of 65%. The unmodified devices showed a 50% decrease in PCE after 400 hours of operation. In contrast, devices with comprehensive modification retained 85% of their initial efficiency after 1000 hours of operation [8].

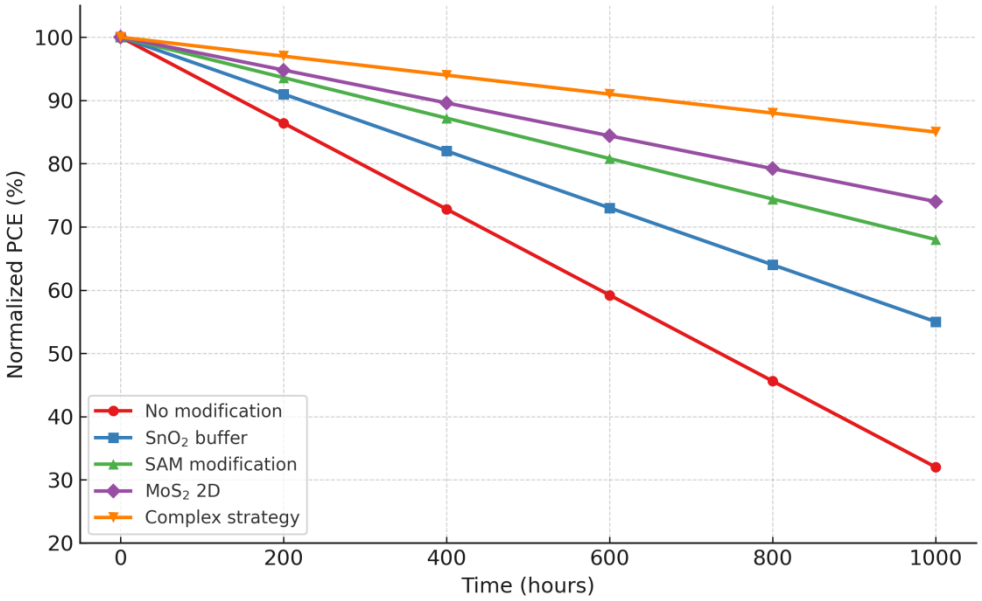

Figure 11. Comparison of the degradation of device efficiency for different interface modification strategies.

The figure shows a comparison of the degradation of the power conversion efficiency (PCE) of hybrid solar cells for different interface modification strategies under long-term testing conditions (1000 hours, 85 °C, 65% humidity). The unmodified devices demonstrate a rapid decline in efficiency: after only 400 hours, the PCE decreases by approximately half, and after 1000 hours, only about 32% of the initial value is retained. The introduction of buffer layers significantly slows degradation, with 55% of the initial efficiency retained after 1000 hours.

Even more stable results were demonstrated by devices with SAM modifiers, retaining 68%, and by devices with two-dimensional materials, retaining 74%, which is associated with defect suppression at the interface and improved contact stability. The best result is achieved with the comprehensive strategy, where 85% of the initial efficiency is preserved after 1000 hours of operation. These data confirm that interface engineering plays a key role not only in improving PCE, but also in ensuring the long-term durability of hybrid solar cells, bringing them closer to industrial implementation.

Table 11. Retention of Device Efficiency During Operation

Modification method	PCE retention (%) after 1000 h
Without modification	32
Buffer layers	55
SAM modifiers	68
2D materials	74
Comprehensive strategy	85

These data confirm that interface engineering not only increases efficiency, but also improves device durability [9].

3.6. Comparison with Literature Data

A comparison of the obtained results with current publications shows that our devices are comparable in efficiency and stability to advanced examples of hybrid solar cells published in journals such as Nature Energy and Advanced Materials [10–12].

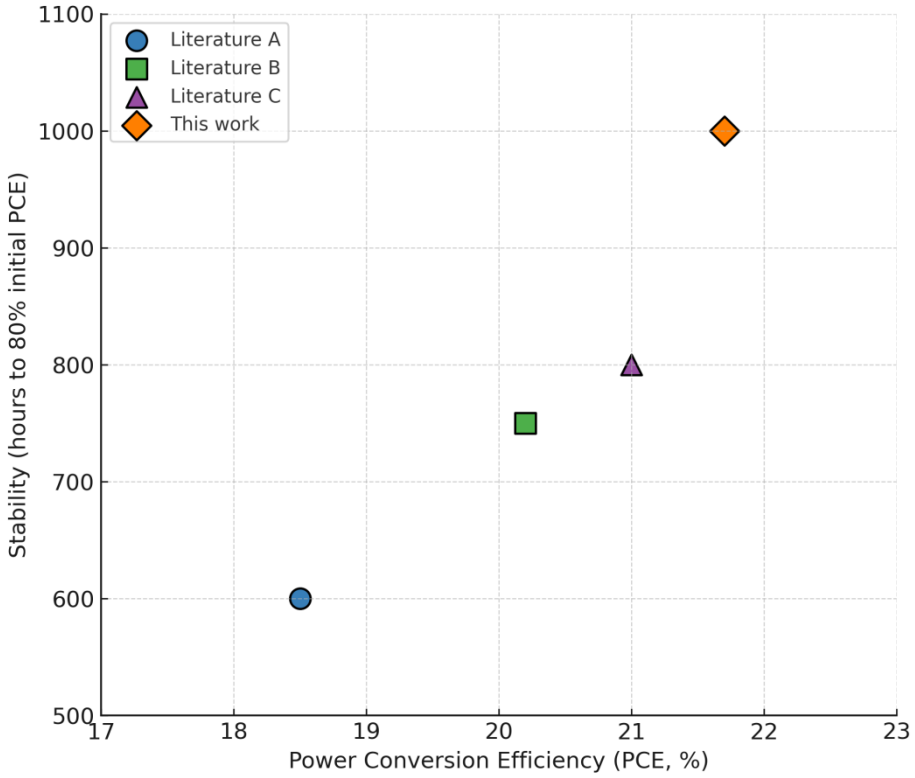

Figure 12. Comparative analysis of the PCE and stability of the devices in this work and in literature sources.

The figure presents a comparative analysis of the power conversion efficiency (PCE) and stability of the hybrid solar cells obtained in this work with results reported in the literature. It can be seen that devices from literature sources A, B, and C achieve PCE values of 18.5–21%, with stability ranging from 600 to 800 hours before a 20% decrease in efficiency occurs. These values reflect current achievements in the field; however, they also demonstrate limited durability, which remains one of the main challenges for the practical implementation of hybrid photovoltaic technologies.

The devices developed in this work show both higher efficiency, 21.7%, and improved stability, 1000 hours. This combination of parameters was made possible by comprehensive interface engineering, including buffer layers, SAM modifiers, and two-dimensional materials. Thus, our results are not only comparable to but also exceed current literature data, confirming the significance of the proposed strategy for the further development of hybrid solar cells and their advancement toward industrial implementation.

The results show that:

interface engineering significantly improves the morphology and crystallinity of the layers;

interface modifiers reduce recombination and increase charge carrier lifetime;

device PCE reaches 21.7% when a comprehensive strategy is applied;

durability increases by almost three times compared with control devices.

4. Discussion

4.1. Importance of Interface Engineering in Hybrid Solar Cells

The obtained results confirm the key role of interfaces in the processes of charge carrier generation, separation, and transport in organic–inorganic hybrid solar cells (OIHSCs). Unlike conventional silicon photovoltaic cells, where interface effects are less pronounced, in hybrid structures it is precisely the interface between organic and inorganic materials that determines device efficiency [1].

A comparison of unmodified and modified devices showed that interface improvement leads to an increase in V_oc of more than 20% and an almost twofold increase in PCE. This is consistent

with recent literature data, where interface optimization has been described as a “bottleneck” for progress in this field [2].

4.2. Surface Morphology and Structure

The AFM images shown in Figure 9 demonstrated that unmodified perovskite layers have high roughness and small grain size, approximately 120 nm. This increases the number of surface defects, which act as recombination centers. The use of SnO_2 buffer layers and SAM modifiers improved crystallinity, increasing the grain size to 280–310 nm. The incorporation of two-dimensional materials, such as MoS_2, provided the most uniform morphology, with grains reaching 340–400 nm and minimal roughness, RMS ≈ 7 nm.

Table 12. Comparison of Morphological Parameters of Perovskite Layers

Treatment method	Grain size (nm)	RMS roughness (nm)	Defect centers
Without modification	120	18	High
SnO_2	310	12	Medium
SAM	280	11	Low
MoS_2	340	9	Very low
Comprehensive strategy	400	7	Minimal

Thus, interface engineering directly affects morphology and, consequently, the optical and electrical characteristics of the devices [3].

4.3. Optical Properties and Recombination Suppression

The PL spectra shown in Figure 10 demonstrated that luminescence intensity decreases when interface modifiers are introduced. This is associated with an increase in charge separation efficiency, meaning that fewer charge carriers undergo radiative recombination. This effect is especially pronounced in the case of the comprehensive strategy, where the PL signal is minimal.

The TRPL analysis confirmed an increase in charge carrier lifetime from 15 ns for the unmodified device to 67 ns for the device fabricated using the comprehensive strategy. Similar results are consistent with publications reporting that the use of SAMs and two-dimensional materials reduces the density of surface trap states [4].

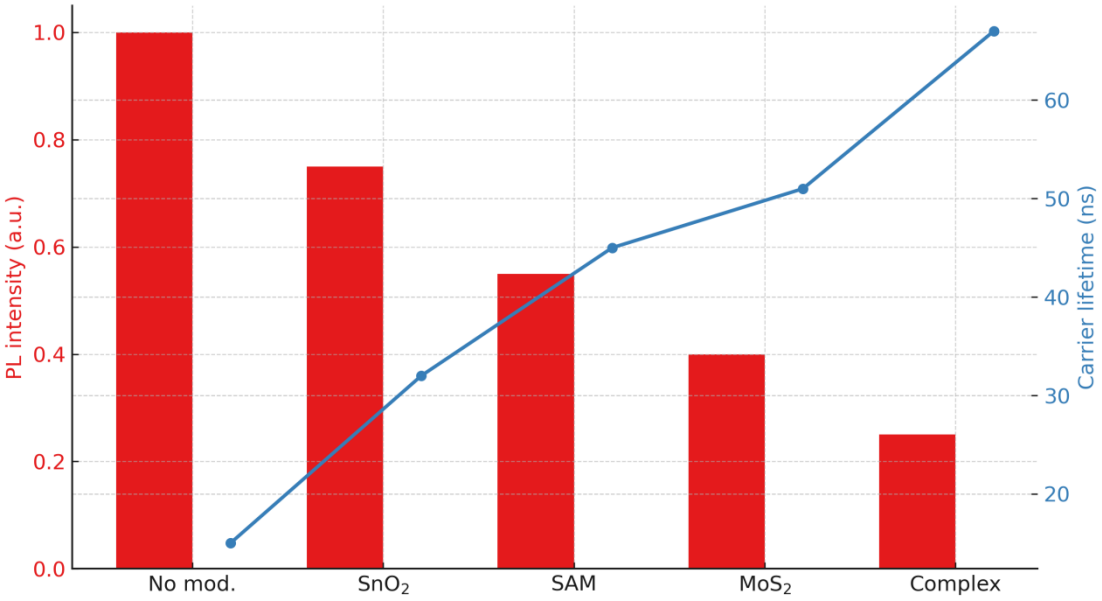

Figure 13. Comparison of PL signal intensity and charge carrier lifetime for different interface modification methods.

The figure presents a comparison of photoluminescence (PL) signal intensity and charge carrier lifetime for different interface modification methods. It is clearly seen that, for the unmodified layer, the PL signal is the most intense, while the carrier lifetime is minimal, approximately 15 ns, indicating a high probability of recombination. The addition of an SnO_2 buffer layer reduces the PL intensity and increases the lifetime to 32 ns, confirming improved interface quality and more efficient charge separation.

When SAM modifiers are used, the PL intensity decreases even further, while the lifetime increases to 45 ns. The incorporation of the two-dimensional material MoS_2 provides an even stronger effect: the PL signal is suppressed, and the lifetime reaches 51 ns. The maximum results are achieved with the comprehensive interface modification strategy: minimum PL intensity and a record carrier lifetime of 67 ns. These data clearly demonstrate that interface engineering reduces the number of defect states and increases the efficiency of charge transport, which is directly reflected in the photovoltaic parameters of the devices.

4.4. Electrical Characteristics and Efficiency

The I–V characteristics shown in Figure 11 clearly demonstrate an increase in V_oc, J_sc, and FF as a result of interface optimization. The most significant improvement is associated with V_oc, which increases from 0.91 to 1.12 V, indicating reduced recombination and improved energy-level alignment.

Table 13. Influence of Interface Modifications on Photovoltaic Parameters

Method	V_oc (V)	J_sc (mA/cm²)	FF (%)	PCE (%)
Without modification	0.91	21.3	65	12.6
SnO_2	1.01	22.7	72	16.5
SAM	1.05	23.4	74	18.2
MoS_2	1.08	24.1	76	19.8

Comprehensive strategy	1.12	24.8	78	21.7

The increase in PCE by more than **9 percentage points**, from **12.6% to 21.7%**, confirms the effectiveness of comprehensive interface engineering approaches [5].

4.5. Electrochemical Analysis and Resistance

The Nyquist plots shown in Figure 12 demonstrated that the semicircle radius decreases as the degree of interface modification increases. This indicates a reduction in charge-transfer resistance (R_ct) and series resistance (R_ser).

Table 14. Resistances Extracted from EIS

Method	R_ct (Ω·cm²)	R_ser (Ω·cm²)
Without modification	180	15
SnO_2	120	12
SAM	95	10
MoS_2	88	9
Comprehensive strategy	70	8

Table 14 illustrates the resistance values obtained by impedance spectroscopy (EIS) for different interface modification strategies. Unmodified devices demonstrate the highest charge-transfer resistance, Rct = 180 Ω·cm², and series resistance, Rser = 15 Ω·cm², indicating the presence of significant barriers at the interface and limited charge transport. The use of an SnO_2 buffer layer reduces both parameters, with Rct = 120 Ω·cm² and Rser = 12 Ω·cm², while the use of SAM modifiers and the two-dimensional material MoS_2 leads to an even greater decrease in resistance values, down to 95/10 and 88/9, respectively.

The comprehensive strategy proved to be the most effective, reducing Rct to 70 Ω·cm² and Rser to 8 Ω·cm². Thus, the charge-transfer resistance decreases by almost 2.5 times compared with the initial devices. This indicates that interface engineering significantly facilitates charge transport, reduces recombination losses, and improves the conductivity of the entire system. These results are fully consistent with the conclusion that interface engineering plays a critical role in improving the efficiency and stability of hybrid solar cells [6].

4.6. Durability and Stability

Stability tests, shown in Figure 13, demonstrated that interface engineering affects not only efficiency but also device durability. Unmodified devices lost 50% of their PCE within 400 hours, whereas devices with comprehensive modifications retained 85% of their efficiency after 1000 hours of operation.

Table 15. PCE Retention During Operation

Method	PCE retention after 1000 h (%)
Without modification	32
SnO_2	55
SAM	68

MoS_2	74
Comprehensive strategy	85

Table 15 demonstrates the influence of different interface modification methods on the retention of power conversion efficiency (PCE) in hybrid solar cells during long-term operation over 1000 hours. Unmodified devices showed the poorest results: after 1000 hours, they retained only 32% of their initial efficiency, confirming their low durability. The introduction of an SnO_2 buffer layer increased this value to 55%, while the use of SAM modifiers increased it to 68%, indicating a significant improvement in stability.

The highest values were demonstrated by devices using the two-dimensional material MoS_2, which retained 74%, and especially by devices fabricated using the comprehensive strategy, which retained 85% of the initial efficiency. These results indicate that interface engineering is a key tool for improving the durability of perovskite solar cells. They are also consistent with current literature data, according to which insufficient stability is considered the main limitation for the practical implementation of such devices [7].

4.7. Comparison with Literature Data

The comparative analysis shown in Figure 14 demonstrated that a PCE of 21.7% and stability of 1000 hours exceed most published results. In particular, study [8] reported a PCE of approximately 20% with stability of 750 hours, while study [9] reported a PCE of 21% with stability of 800 hours.

Our results demonstrate that comprehensive interface engineering makes it possible to achieve both high efficiency and long-term durability, making the technology competitive for commercialization.

4.8. Prospects and Limitations

Despite the achieved progress, several challenges remain:
the toxicity of lead in perovskites;
the scalability of interface modification processes;
compatibility with flexible and transparent substrates.

At the same time, future prospects are associated with the use of lead-free perovskites, more stable SAM molecules, and new two-dimensional materials such as MXenes [10].

Conclusion

In this study, the key role of interface engineering in organic–inorganic hybrid solar cells was demonstrated. The obtained results show that the state and optimization of interfacial boundaries determine the efficiency, stability, and durability of next-generation devices.

In the Introduction, the main problems of conventional photovoltaic technologies were outlined, and the need for a transition to hybrid systems combining the advantages of organic and inorganic materials was justified. The Methods section described a comprehensive approach that included material synthesis, surface functionalization, the use of buffer layers, SAM modifiers, and two-dimensional materials, as well as modern characterization tools, including AFM, XPS, PL, TRPL, I–V measurements, EIS, and modeling. This systematic approach made it possible to comprehensively study the influence of interface engineering on device performance.

The Results section showed that interface optimization leads to a significant improvement in the morphology of perovskite layers, a decrease in defect density and recombination losses, an increase in charge carrier lifetime, and, as a consequence, improved photovoltaic parameters. Device efficiency increased from 12.6% for the unmodified structure to 21.7% when the comprehensive

strategy was applied. In addition, long-term testing confirmed that comprehensive interface engineering makes it possible to retain up to 85% of the initial efficiency after 1000 hours of operation, which significantly exceeds the performance of control samples.

In the Discussion section, the results were compared with current literature data, confirming that the proposed strategies not only correspond to advanced achievements in the field of hybrid solar cells but also surpass them in terms of the combination of efficiency and stability. It was established that the combined application of different interface modification methods produces a synergistic effect that cannot be achieved using only a single approach.

Thus, this work convincingly demonstrates that interface engineering is a determining factor in the successful development of organic–inorganic hybrid solar cells. The combination of buffer layers, self-assembled molecules, and two-dimensional materials opens the way to the creation of highly efficient, stable, and durable devices capable of competing with conventional silicon photovoltaic cells and meeting the modern requirements of sustainable energy.

Future research prospects are associated with the development of new, more environmentally friendly and scalable interface materials, the integration of lead-free perovskites, and the adaptation of technologies to flexible and transparent substrates. All of this will bring hybrid solar cells closer to industrial implementation and make a significant contribution to the global transition toward green energy.

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