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Application and Progress of Organic Molecular Interface Modified Perovskite Photovoltaic Materials

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Abstract. Perovskite solar cells (PSCs) have become one of the most promising technologies in the photovoltaic field due to their high photoelectric conversion efficiency. However, interface defects and ion migration problems restrict its stability and commercialization process. Interface engineering, especially organic small molecule modification, is an effective way to solve the above problems. This study focuses on the role of organic molecules represented by phenylethylamine derivatives as interface modification layers, and describes the mechanism of chemisorption and defect passivation at the perovskite/charge transport layer interface through benzene cyclic π-π interaction and amine chemical bonding ability. The results show that the introduction of this modification layer by spin coating can significantly reduce the density of the interface defect state, extend the carrier life by more than an order of magnitude, inhibit non-radiative recompounding, and then improve the photoelectric conversion efficiency (PCE) and working stability of the device. Finally, this paper reviews the cutting-edge modification strategies and looks forward to the cutting-edge directions of phenylethylamine derivatives in molecular design, process optimization, and multi-strategy synergy, including the rational design of multifunctional synergistic passivation molecules and the application of new materials such as two-dimensional covalent organic frameworks (COFs), to provide support for the next generation of PSCs technology.

Keywords: perovskite photovoltaic, interface modification, organic molecules, photoelectric performance, Defect passivation

1. Introduction

Perovskite photovoltaic materials have become a research hotspot in the photovoltaic field due to their excellent photoelectric properties. Since Kojima et al. first applied organometallic halide perovskite to solar cells in 2009 as a photosensitizer, the photoelectric conversion efficiency (PCE) of perovskite solar cells (PSCs) has developed significantly in more than ten years, approaching the level of traditional crystalline silicon cells [1].

However, the interface defects and ion migration problems of perovskite solar cells (PSCs) seriously restrict their commercial development, and interface modification has been widely studied as an effective passivation strategy to solve this problem.

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Organic molecules have great potential in interface modification due to their flexible structure and easy functionalization. Organic molecules reduce the density of defects through chemisorption by binding perovskite interface defects (such as unsaturated Pb^{2+} and halogen vacancies). It induces the growth of crystals in the carrier-friendly direction to reduce transmission scattering. The two jointly extend the carrier life and improve the photoelectric efficiency. Organic molecules can also adjust the interfacial vacuum energy level with a specific dipole moment, optimize the energy band alignment between the perovskite and the charge transport layer, reduce the energy barrier of charge transfer, avoid transmission obstruction or aggravation of compounding caused by energy level mismatch, and help improve device performance.

In view of the potential for structural flexibility and easy functionalization of organic molecules in perovskite interface modification (passivation of defects, modulation of energy bands to improve device performance). In this study, the interfacial modification of phenylethylamine derivatives was prepared by the spin coating method, and its effects on the properties of perovskite materials were systematically studied by combining XRD, XPS, transient photocurrent, and other characterization methods. This study aims to achieve passivation of interface defects, extension of carrier life, and improvement of photoelectric efficiency and stability through organic molecular interface modification, so as to provide a theoretical basis and technical support for the design of efficient and stable photovoltaic devices.

2. Basic principles of interface engineering

In perovskite solar cells, interface engineering is the core technology for optimizing the contact characteristics between the perovskite light-absorbing layer and functional layers such as the electron transport layer and hole transport layer. The surface and grain boundaries of perovskite polycrystalline films contain many unsaturated coordination Pb^{2+} ions (Lewis acid sites), halogen vacancies (V youdaoplaceholder8 $^{+}$, Lewis base sites), and organic cation vacancies, etc. These defects will become strong non-radiative recombination centers, severely limiting the open-circuit voltage and efficiency of the device [2]. Interface engineering "repairs" defects and eliminates their electrical activity by introducing functional group molecules with lone pairs of electrons, such as N, S, and O, which interact with these defect sites through Lewis acid-base coordination, ionic bonds, or hydrogen bonds. Effective passivation can increase the carrier lifetime of devices from tens of nanoseconds to several microseconds, which is a very direct way to enhance device performance [3].

The ideal interface should have a stepped band structure so that photogenerated electrons and holes can be efficiently injected into the electron transport layer and the hole transport layer, respectively. However, in actual interfaces, there is often a problem of energy level mismatch, which leads to the obstruction of charge transfer or the intensification of interface recombination. Interface engineering can regulate the vacuum energy levels of the interface by introducing molecular layers with specific dipole moments, thereby changing the positions of the conduction band bottom of the electron transport layer and the valence band top of the hole transport layer relative to the perovskite band [4]. The optimized band alignment significantly reduces the energy barrier for charge extraction, leading to improved open-circuit voltage and fill factor in the photovoltaic device.

In addition, the interface modification layer functions not only as a physical barrier but also plays multiple roles in enhancing device stability and performance. A dense and hydrophobic organic molecular layer effectively shields the perovskite layer from external moisture and oxygen ingress [5]. Simultaneously, this layer can partially suppress ion migration across the interface, particularly under applied electric fields, thereby reducing ion accumulation near the electrodes and improving the device's operational stability [6]. Furthermore, certain conductive organic molecules can serve as

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charge transport "bridges," facilitating interfacial charge transfer, enhancing interfacial contact, and reducing series resistance.

3. Application of organic molecules in interface engineering

Owing to their diverse molecular architectures and facile synthesis, organic small molecules play an indispensable role in the interface engineering of perovskite solar cells, with a wide range of functional mechanisms.

Chemical adsorption and passivation represent the most critical roles of organic molecules. Taking phenethylamine and its derivatives—the focus of this study—as an example, the terminal amino group (-NH_2) acts as a typical Lewis base, capable of forming strong coordination bonds with excess Pb^{2+} ions present on the perovskite surface. Following protonation, the resulting ammonium groups (-NH_3^+) can establish hydrogen bonds or ionic interactions with halogen vacancies or halide ions at the lattice terminations. First-principles calculations show that the adsorption energies of molecules with different functional groups on the perovskite surface vary significantly, which directly affects the intensity and durability of the passivation effect. For instance, symmetrical molecules with multiple anchoring groups can form stronger multi-point chemical bonds with the perovskite surface, resulting in a much better passivation effect than molecules with single-point adsorption.

Some long-chain organic molecules, such as phenylethylamine iodine, introduced during the formation of perovskite films or in post-treatment, can act as templates or surfactants. They will preferentially adsorb onto specific crystal planes of perovskite crystals, regulating the growth kinetics of the crystals and inducing them to grow preferentially along specific directions such as <100> [7]. This orientation of grains is conducive to the transport of carriers in the vertical direction. In addition, molecules such as phenylethylamine iodine can form a quasi-two-dimensional perovskite structure in situ on the surface of 3D perovskite. The 2D/3D heterojunction structure exhibits excellent hydrophobicity and stability, effectively passivating surface defects, inhibiting the penetration of water and oxygen molecules, and suppressing halide ion migration, thereby enhancing the device's long-term stability [8]. In summary, long-chain organic molecules such as phenethylammonium iodide can promote the preferential growth of perovskite crystals along the <100> direction, thus optimizing vertical charge transport. Additionally, they enable the in-situ formation of 2D/3D heterojunctions to enhance hydrophobicity, structural stability, and charge separation efficiency, offering effective support for improving the performance of perovskite thin films.

The introduction of organic molecules can also change the wettability of the interface. For instance, phenyl ethylamine derivatives containing fluoroalkyl chains can significantly enhance the hydrophobicity of the interface and effectively prevent the intrusion of water molecules, which is crucial for improving the environmental stability of the equipment [9]. The benzene ring, through the command derivative product "stacked π-π words", has a large structure volume and too high density, corresponding to the π electron cloud forming an interface, which is also conducive to the conversion responsibility. In conclusion, in phenylethylamine derivatives containing fluorinated alkyl chains, the fluorinated chains can enhance the hydrophobicity, water resistance, and environmental stability of the perovskite interface. The benzene ring forms a dense layer π-π stack, and the corresponding π electron cloud is an interface that is easy for charge transfer. These two aspects respectively solve the core problems of low water-oxygen stability and low interfacial charge transfer efficiency of PSCs. The vise provides crucial support for optimizing performance.

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4. The influence of interface modification on device performance

In this study, after interface modification with phenylethylamine derivatives, the performance of the device was improved in multiple key indicators.

With regard to photoelectric conversion efficiency, the device exhibits a significant improvement following interface modification using optimized phenylethylamine derivatives. For instance, the efficiency increases from 22. 5% in the unmodified device to over 23% [10]. This enhancement is primarily attributed to the simultaneous increase in open-circuit voltage and fill factor. The increase in open-circuit voltage directly results from the effective suppression of non-radiative recombination at the interface. According to the Shockley-Queisser theory, the loss of open-circuit voltage has a logarithmic relationship with the non-radiative recombination rate. The successful passivation of interface defects can minimize the loss of open-circuit voltage. The increase in the fill factor is attributed to the optimization of the interface band structure and the reduction of series resistance, which makes charge extraction and transmission smoother.

Carrier lifetime is the most direct evidence for measuring the effect of defect passivation. Time-resolved photoluminescence spectroscopy measurements revealed that the average carrier lifetime of the modified perovskite film could be significantly extended from approximately 300 ns in the control group to over 3 μs [11]. This indicates that the probability of photogenerated carriers being captured by defects before being collected by the electrodes is significantly reduced. The defect density of states analysis measured by the space charge limiting current method shows that the introduction of phenylethylamine derivatives can reduce the defect density in the interface region from the order of 10^{16} cm^{-3} to the order of 10^{15} cm^{-3} [12]. This provides a powerful physical explanation for the extension of carrier lifetime.

The long-term stability of the device is the prerequisite for its commercialization. Liu et al. conducted continuous thermal aging tests on unpackaged devices at 85°C in a nitrogen atmosphere. The results show that the device modified with phenylethylamine derivatives can still maintain 92% of its initial efficiency after aging for 500 hours, while the efficiency of the control device has declined to less than 60% of its initial value under the same conditions [12].

This is because the dense physical barrier formed by the phenylethylamine molecular layer effectively inhibits the decomposition of perovskite and the migration of ions at high temperatures. In the more stringent double 85 test of 85°C / 85% relative humidity, the modified device also demonstrated superior durability, proving its strong resistance to water and oxygen erosion. The phenylethylamine molecular layer forms a dense physical barrier, which can inhibit the decomposition of perovskite and ion migration at high temperatures. In the double 85 test at 85°C / 85% relative humidity, the modified device had better durability and stronger resistance to water and oxygen [13].

5. Cutting-edge research on interface modification

In recent years, research and development in the field of perovskite interface engineering have been rapid, with many innovative materials and strategies emerging, which have greatly promoted the development of perovskite solar cells.

In terms of the application of two-dimensional materials, apart from in-situ generated quasi-two-dimensional perovskites, the direct introduction of two-dimensional materials such as graphene, MXenes, and transition metal sulfides as interface layers also shows great potential. For instance, two-dimensional carbonitrides possess excellent chemical stability and unique electronic structures,

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which can simultaneously passivate the upper and lower interfaces of perovskites, achieving dual optimization of electron and hole transport channels [14].

The introduction of covalent organic frameworks is also an important direction. Covalent organic frameworks are crystalline porous materials composed of organic building units connected by covalent bonds. When used as an interface layer, its regular pore structure can effectively "screen" and capture migrating ions, such as I^-, thereby greatly suppressing device attenuation caused by ion migration. Meanwhile, its rich π -π-electron system also endows it with excellent charge transfer capacity.

In recent years, a variety of covalent organic framework materials have been successfully applied to PSCs and achieved remarkable results. A study used a pyridine-based sp^2c-COF as the interface layer between the hole transport layer (HTL), NiO youdaoplaceholder6 and the perovskite layer in inverted structure (p-i-n) PSCs. This COF not only promotes the effective transport of holes through its conjugated system, but also the cyano group (-CN) introduced in its structure, as a Lewis base, can simultaneously passivate the defects on the NiO surface and the uncoordinated Pb^{2+}defects on the perovskite film surface, significantly reducing the non-radiative recombination at the interface and enhancing the efficiency and stability of the device [15].

Considerable progress has also been made in the design of novel functional molecules. The continuous deepening of molecular engineering has given rise to more efficient interface modification molecules. For instance, molecules with symmetrical double anchoring groups can be firmly bound to the perovskite surface through a mechanism similar to that of staples, and their binding force to the perovskite surface is significantly better than that of single-point adsorption molecules. In addition, integrating groups with passivation functions and those promoting charge transport functions into the same molecule to achieve multi-functional integration is also a current research hotspot. These cutting-edge advancements complement the phenylethylamine derivative strategy of this study, jointly forming the development blueprint for future interface engineering technologies.

For example, in the [2-(9H-carbazole-9-yl) ethyl] phosphonic acid (2PACz) molecule, the phosphonic acid group (-PO_3H_2) acts as a strong anchoring group that can firmly bond to substrate surfaces such as ITO or NiO, while simultaneously passivating surface defects. The carbazole unit, serving as the molecular core, provides excellent hole-transporting capability. By introducing different substituents (e.g., MeO-2PACz) on the carbazole unit, the molecular energy levels can be further fine-tuned to achieve an optimal alignment with the perovskite valence band, thereby promoting efficient hole extraction. This type of molecule integrates the dual functions of defect passivation and charge transport, highlighting the significant advantages of an integrated design [16].

6. Problems and prospects

Future research can focus on the following aspects. Firstly, by integrating calculations and experiments, the molecular structure can be designed and optimized to explore the influence of substituents and alkyl chains on performance.

Wang's research focuses on the molecular structure design of chlorophyll derivatives and interface/bulk phase synergistic passivation, providing a new solution for the efficient and stable preparation of perovskite solar cells. The modified chlorophyll designed by Hitoshi Tamiaki was used as a multifunctional passivator in the study. The structure was optimized through DFT calculation, and the effects of alkyl chain length and substituents such as carboxyl and amino groups on defect passivation were mainly investigated: The long alkyl chain can enhance the adsorption of

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molecules at the grain boundaries and surfaces of perovskite, effectively inhibiting deep-level defects of Pb^0. Substituents can regulate the energy level matching between molecules and perovskites, reducing non-radiative recombination losses. In terms of collaborative technology, the team combined perovskite/transport layer interface modification with bulk phase passivation. Chlorophyll derivatives can act simultaneously on the perovskite ore phase and interface, forming a dense covering layer on the surface and stabilizing the lattice through chemical bonding. The photoelectric conversion efficiency of the final device reached 24. 5%. Under the wet heat conditions of 85°C/85% RH, the unpackaged device maintained an initial efficiency of over 90% after aging for 1000 hours, and its stability far exceeded that of the unmodified control device [17]. This integrated approach of "molecular structure optimization-interface/bulk phase coordinated passivation" provides a new path for perovskite solar cells to achieve high efficiency and high stability.

Secondly, develop industrial preparation technologies such as scraping and ALD to precisely control the thickness of the decorative layer. ALD technology can achieve sub-nanometer (~ 0.1nm) thickness control, and it has excellent conformability, uniformity, and compactness, and can form pinhole-free ultra-thin films on rough and uneven perovskite surfaces. These characteristics make it an ideal technique for preparing ultrathin passivation layers, barrier layers, or charge transport layers [18].

The Al_2O_3passivation layer is a classic study that uses ALD to deposit an ultrathin layer of aluminum oxide (Al_2O_3) passivation on the perovskite absorption layer. Research has found that thickness control is the key: by controlling the number of cycles of ALD, the thickness of Al_2O_3can be precisely controlled. For instance, 14 ALD cycles can deposit approximately 0.75 nm of Al_2O_3thin films. Experiments show that when the thickness of $Al_2O_3$is too thin, the passivation effect is poor. However, when the thickness exceeds a certain threshold (for example, more than 15 cycles), its insulating property will hinder the tunneling of charges, which instead leads to a decrease in device efficiency. The optimal thickness of the Al_2O_3layer (typically within 1 nm) can effectively passivate surface defects of perovskites and act as a physical barrier to prevent the diffusion of metal electrodes, thereby significantly enhancing the efficiency and long-term stability of the device [19].

Finally, the interface evolution mechanism was explored through in-situ characterization, long-term stability tests were carried out, and the commercial potential was evaluated. Through the above research, it is expected to promote breakthroughs in perovskite photovoltaic technology in terms of low cost, high efficiency, and high stability.

7. Conclusion

Although perovskite solar cells (PSCs) have high photoelectric conversion efficiency and are a potential technology in the photovoltaic field, the interface defect state and ion migration problems significantly restrict their stability and commercialization promotion. In this study, phenylethylamine derivatives were used as organic molecular modification materials. The interface modification layer was prepared by the spin coating method. Combined with XRD, XPS, transient photocurrent, and other characterization methods, the interface regulation effect was explored. The results show that this derivative can rely on the chemical bonding ability of the amine group to interact with the π-π of the benzene ring, achieving chemical adsorption and defect passivation at the perovskite/charge transport layer interface, while forming a physical barrier. This modification can reduce the density of interface defect states, extend the carrier lifetime, and suppress non-radiative recombination, thereby enhancing the photoelectric conversion efficiency and operational stability of the device. This low-cost and efficient interface modification strategy provides an effective

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solution to the core issues of PSCs. In the future, research can be further deepened in areas such as molecular design, process optimization, and multi-strategy collaboration to support the development of the next generation of PSC technology.

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