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Interfacial Defect Passivation in Perovskite Solar Cells: A Molecular and Chemical Perspective

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ABSTRACT

Interfacial defects that control non-radiative recombination, ion migration, and long-term instability have limited the commercialization of metal halide perovskite solar cells (PSCs), which have achieved remarkable laboratory-scale power conversion efficiencies (PCEs) approaching 27%. Although substantial research has focused on defect passivation, studies have remained largely material-specific and empirical and lack a unified understanding of the chemical interactions occurring during defect passivation. This paper provides a molecular-level chemical perspective on interfacial defect passivation in PSCs. The electronic and ionic contributions to the nature and origin of interfacial defects, such as undercoordinated Pb^{2+} ions, halides, and organic cation deficiencies, are systematically discussed. The primary passivation mechanisms, like Lewis acid-base coordination, ionic compensation, hydrogen bonding, coordination chemistry, and dipole-induced field effects, are critically examined in terms of their contribution to the modulation of defect energetics and charge dynamics. Interface-specific phenomena at the perovskite/electron transport layer, perovskite/hole transport layer, and buried interfaces are also discussed to highlight the need for specific passivation methods. This paper provides a unified overview of rational interface design and offers insights into the development of stable, highly efficient, and scalable PSC technologies.

Keywords: halide vacancies, open-circuit voltage (V_{oc}), defect passivation, hysteresis, interfacial layers

1. INTRODUCTION

Metal halide perovskite solar cells (PSCs) have emerged as a promising advancement in photovoltaic technology because of their exceptional photoelectronic properties, including high absorption coefficients, tunable bandgaps, and extended carrier diffusion lengths. In recent years, PSCs have progressed rapidly, with power conversion efficiencies (PCEs) now exceeding 26% and approaching those of conventional crystalline silicon solar cells [1–3]. However, the large-scale commercialization of PSCs remains constrained by limitations in device reliability and durability. A growing body of evidence suggests that these constraints are primarily driven by defects, particularly those at the interface between the perovskite absorber and charge transport layers [4,5]. Point defects, such as undercoordinated ions and halide vacancies, can arise from structural discontinuities and chemical incompatibilities at these interfaces. These defects can act as non-radiative recombination centers, thereby lowering the open-circuit voltage (V_{oc}) and overall device efficiency [6]. Moreover, interfacial defects can facilitate ion movement and promote degradation under environmental stresses such as heat, light, and moisture. Therefore, interface engineering is critical for improving the performance and stability of PSCs, as illustrated in Figure 1 [7].

These problems have been addressed using a wide variety of defect passivation methods, including interfacial layers, additives, and surface treatments [8,9]. However, most existing studies and reviews have focused primarily on the classification of material systems or fabrication techniques, while defect passivation strategies have been largely treated as an empirical process. These approaches fail to recognize the importance of the chemical interactions at the molecular scale, which determine the formation, evolution, and passivation of interfacial defects. Recent studies have shown that the primary physical mechanisms governing passivation efficiency include Lewis acid-base coordination, ionic compensation, hydrogen bonding, and dipole-induced electrostatic effects, which directly influence charge-recombination dynamics and energy-level alignment [10,11]. However, this progress has not yet led to the establishment of a well-defined and consistent relationship between molecular interactions and device-level performance.

Furthermore, the chemistry of buried interfaces remains poorly understood because these interfaces are more difficult to investigate experimentally than the other interfaces, despite being critical to long-term operational stability [2]. The relationship between defect passivation and charge transport is also complex and has not been fully understood, with many passivation strategies introducing barriers to carrier extraction.

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These knowledge gaps highlight the need for more comprehensive, chemically-based insights into interfacial defect passivation. Within this framework, the present article adopts molecular and chemical perspectives to analyze the origins of interfacial defects, elucidate the underlying mechanism of defect passivation, and establish clear relationships between interfacial chemistry and photovoltaic performance. This review seeks to provide a comprehensive framework for the rational design of stable, high-efficiency PSCs by focusing on interaction-driven rather than material-specific processes.

2. ORIGIN AND NATURE OF INTERFACIAL DEFECTS

The performance limitations of PSCs are increasingly thought to arise not due to bulk defects, but rather due to the thermodynamically and chemically heterogeneous nature of the interfaces, where defect formation is thermodynamically favored and kinetically accelerated. Unlike bulk defects, interfacial defects are strongly influenced by abrupt discontinuities in the crystal lattice and chemical mismatches between the perovskite absorber and the surrounding charge transport layers. These characteristics result in a high density of electronically active defect states that strongly influence charge-carrier recombination pathways [2,4]. Notably, both experimental and theoretical studies have shown that when bulk defect densities are minimized, interfacial defect formation becomes rate-limiting, thereby limiting device efficiency.

From the chemical perspective, one of the most prevalent interfacial defect species is the undercoordinated Pb^{2+} ion. This defect arises from incomplete octahedral coordination of Pb atoms at the surface and interface Figure 2. These uncoordinated Pb^{2+} centers are strong Lewis acids and introduce trap states within the bandgap. These traps can act as effective recombination centers by capturing photogenerated electrons and facilitating undesirable recombination. The concentration of these defects is nonuniform and strongly depends on the conditions under which the interface is formed, particularly the quality of contact with the transport layers and the extent of surface coverage. Inadequate contact or surface coverage can increase the population of undercoordinated interfaces [10]. Consequently, devices with similar bulk crystallinity can exhibit substantially different efficiencies because of variations in interface quality.

Halide vacancies represent another important class of defects and play a fundamental role in electronic and ionic processes. They often form during film formation through halide volatilization or incomplete precursor conversion, and their concentration may increase further under operational stress. In contrast to Pb-related defects, halide vacancies are highly mobile and provide major pathways for ion movement. Consequently, the interfacial defect population is not static but can evolve under an electric field or illumination. Halide vacancies are therefore closely associated with current–voltage hysteresis and time-dependent instability, with their defect chemistry directly influencing the time-dependent behavior of devices [6,11].

Organic cation vacancies (MA^+, FA^+), which alter the structural and electrostatic environment at an interface, represent another class of interfacial defects that has received less attention but is increasingly recognized as significant. The loss of these cations can cause localized lattice distortions and alter the hydrogen-bonding network, thereby destabilizing the perovskite framework. More importantly, these vacancies may promote defect-coupling mechanisms that form complex defect structures with enhanced recombination activity. Thus, interfacial defects may not exist independently but can interact with one another,

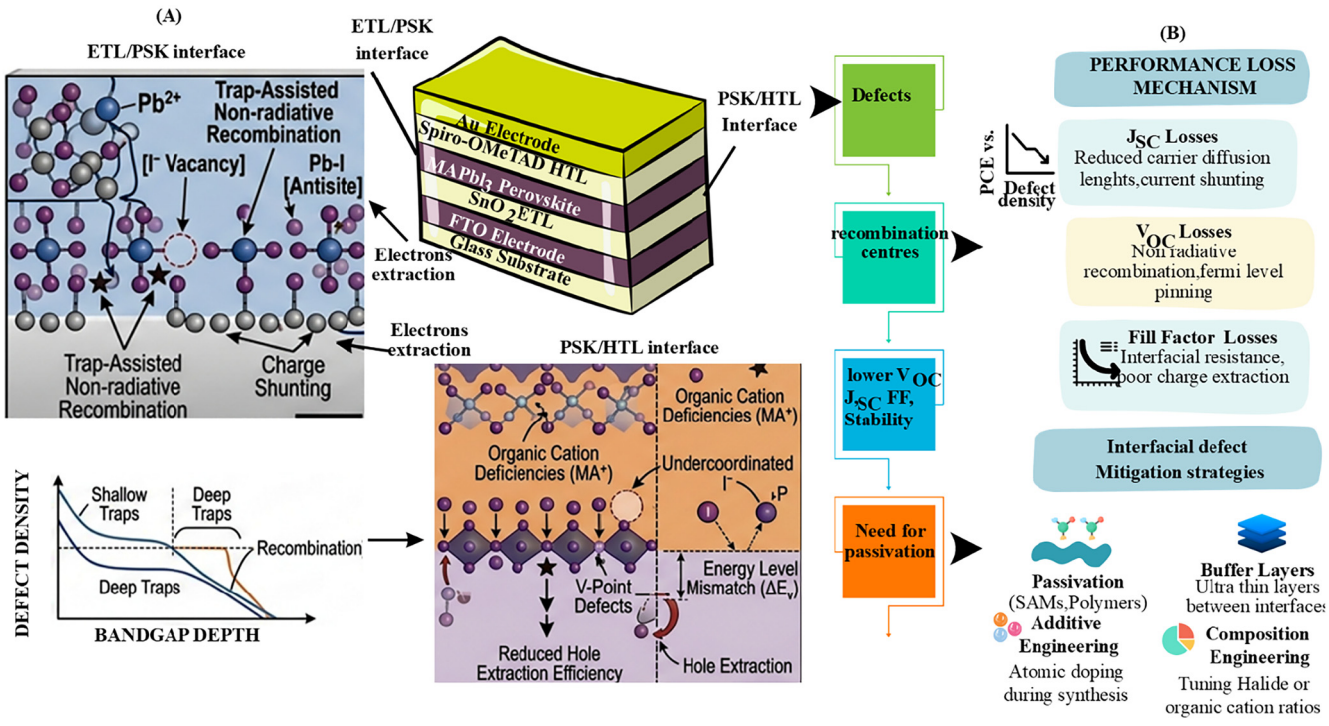

Figure 1. Understanding interfacial defects in PSC devices: (a) Atomic-scale interfacial defect identification, including undercoordinated ions and vacancies; (b) impact on device performance, charge recombination, migration, and mitigation of these defects

highlighting the interconnected roles of chemical and structural factors [7,12].

Chemical defects are dynamic and depend on both processing parameters and environmental exposure. The initial conditions of defect formation are determined by factors such as the crystal growth rate, residual solvents, and energy mismatch at the interface between crystalline and non-crystalline materials. However, chemical reactions and ion redistribution can continue to generate additional defects during subsequent degradation or defect evolution caused by environmental exposure, such as exposure to air or moisture and thermal stress [13]. These different defect-formation conditions can result in substantial differences in device behavior. Consequently, defects at crystalline interfaces do not affect device performance solely thought carrier trapping and recombination. Three processes associated with these defects are particularly important: carrier recombination, ion migration, and interfacial energetics. First, defect-trap states reduce carrier lifetimes and promote non-radiative recombination, thereby reducing the open-circuit voltage (V_{oc}). Second, mobile defects, such as halide vacancies, can create spatially nonuniform electric fields and contribute to hysteresis. Third, defect-induced perturbations at interface can alter band alignment and create potential barriers to efficient carrier extraction [1].

These effects co-exist, demonstrating that interfacial defects are not merely passive imperfections but play an active role in determining device physics. The nature and origin of interfacial defects in PSCs are highly complex and involve intricate interactions that depend on chemical bonding to other materials, structural disorder/defect density in space, and their relationship and/or interaction with the immediate environment(s). Understanding the interplay among these factors is critical for developing rational defect-passivation strategies. For example, undercoordinated Pb ions and halide vacancies are highly chemically reactive, highlighting the need for passivation strategies that specifically address molecular-level interactions (e.g., eliminating or chemically modifying undercoordinated Pb ions) rather than relying solely on physical encapsulation or empirical material properties.

3. CHEMICAL MECHANISMS OF INTERFACIAL DEFECT PASSIVATION

The effectiveness of defect passivation depends on the nature of the chemical interactions between the passivator and the defect site. Modern passivation extends beyond surface modification and involves molecular-level interactions that can modulate the electronic structure, defect energetics, and interfacial charge transfer, thereby enabling more effective defect passivation. Passivation mechanisms can generally be grouped into five main categories: Lewis acid-base interactions, ionic compensation, hydrogen bonding, coordination chemistry, and dipole-induced field effects. Notably, these mechanisms can coexist and act synergistically to suppress defects and enhance performance (Figure 3 and Table 1).

3.1. Lewis Acid–Base Interactions. One of the most common approaches to passivating interfacial defects involves Lewis acid–base interactions, particularly between undercoordinated Pb^{2+} ions and electron-donating molecules. The uncoordinated environment at the perovskite interface renders Pb^{2+} ions strong Lewis acids, which can be easily attacked by nucleophilic species. Molecules containing lone-pair donor groups, such as amines (–NH2), thiols (–SH), and phosphines, can donate electron density to these trap sites and form coordination bonds. These interactions can reduce the density of deep-level

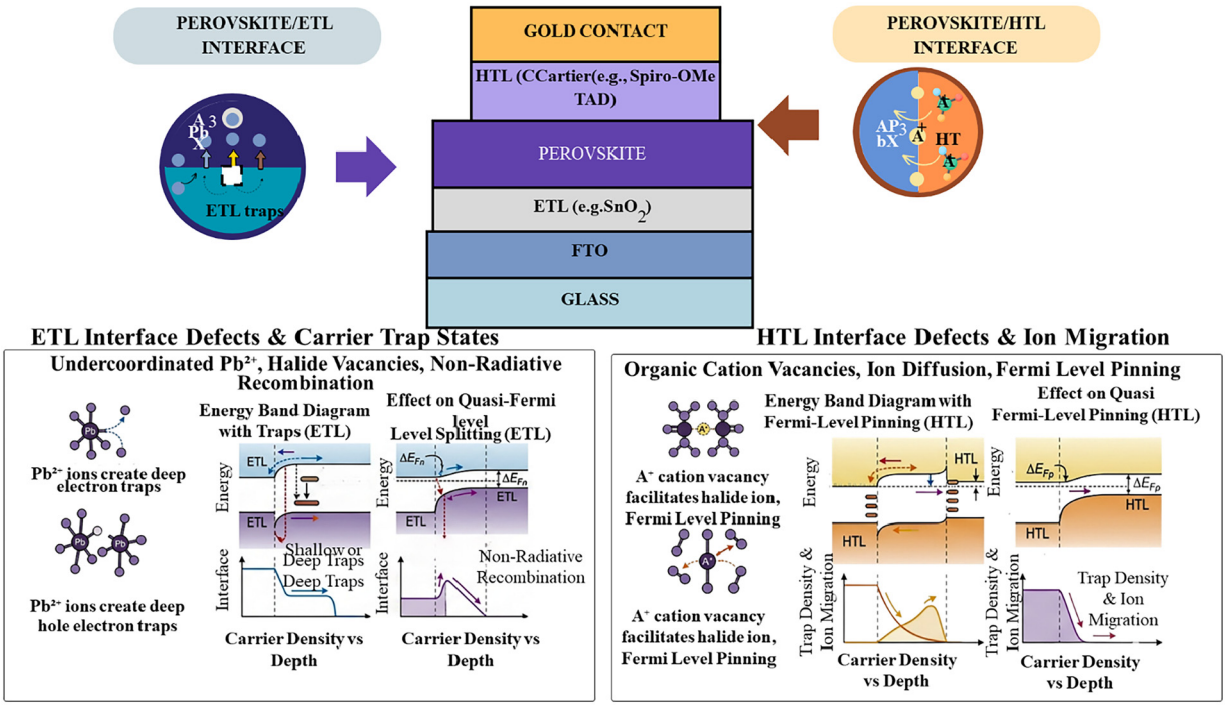

Figure 2. Schematic illustration of different types of interfacial defects and their electronic effects at perovskite/ETL and perovskite/HTL interfaces in PSCs, including their influence on charge extraction, recombination, and trap-state formation

traps, thereby suppressing nonradiative recombination pathways and increasing V_{oc}. In particular, the strength and stability of interactions with the Pb^{2+} group depend on the identity and polarizability of the donor atoms as well as on the molecular structure of the passivating compounds [14,15]. However, a critical balance between the passivation strength and electronic coupling must be maintained because highly strong passivation may impede charge transfer. Recent studies also indicate that passivating agents of both dipole formation and Lewis-base interactions can exhibit high passivation efficiencies, highlighting the importance of molecular-level passivator design [16,17]. Lewis acid–base interactions are among the most common mechanisms for passivating undercoordinated metal ions through chemical coordination. However, other defects, particularly mobile ionic vacancies, require complementary passivation mechanisms such as ionic compensation, as discussed in the next section.

3.2. Ionic Compensation. Another complementary approach to passivating vacancy defects is ionic compensation, in which vacancy defects are filled by mobile ions, primarily halide ions. These vacancies often form during film processing or environmental exposure, creating trap states and facilitating ion migration. Local stoichiometry can be restored and defect density reduced by adding halide salts (KI, FAI, or MACl) to the mixture, including MACl in dilute solutions. Ionic passivation stabilizes the crystal lattice through two primary mechanisms: reducing local charge imbalances and decreasing defect formation energy. These mechanisms can result in two beneficial effects : longer carrier lifetime and reduced hysteresis. However, the effectiveness of this approach depends strongly on ion mobility and distribution; excess ion incorporation can induce phase separation and/or alter the crystallization behavior [18,19]. Furthermore, ionic compensation can alter local electric fields at the interface and thereby affect whether charge extraction. Therefore, ionic passivation involves both structural and electrochemical factors that must be carefully controlled to maximize device performance. In addition to restoring ionic stoichiometry, stabilizing the perovskite lattice is critical. Hydrogen-bonding interactions provide another mechanism for stabilizing interfaces and inhibiting defect evolution.

3.3. Hydrogen Bonding. Although relatively weak, hydrogen bonding plays an important role in stabilizing perovskites interfaces, particularly those containing organic cations like methylammonium (MA^+) or formamidinium (FA^+) cations. Passivating agents containing functional groups such as -NH, -OH, or -COOH can form hydrogen bonds with halide ions or organic cations, thereby enhancing the structural stability of the perovskite lattice. These interactions can reduce lattice distortion and thereby suppress defect formation, particularly under environmental stress. Furthermore, hydrogen bonding can improve moisture resistance by forming a protective network that limits water penetration and subsequent hydrolysis reactions. Hydrogen-bonded interfacial layers have been shown to significantly improve device stability under humid conditions without altering the electronic properties of materials [20,21]. Unlike strong coordination bonds, hydrogen bonds are dynamic and reversible and can therefore provide both structural adaptability and defect passivation. These characteristics can contribute to improved long-term operational stability. Although hydrogen-bonding interactions are relatively weak and reversible, stronger and more persistent defect passivation can be achieved though coordination chemistry involving multidentate ligands. This is discussed in the next section.

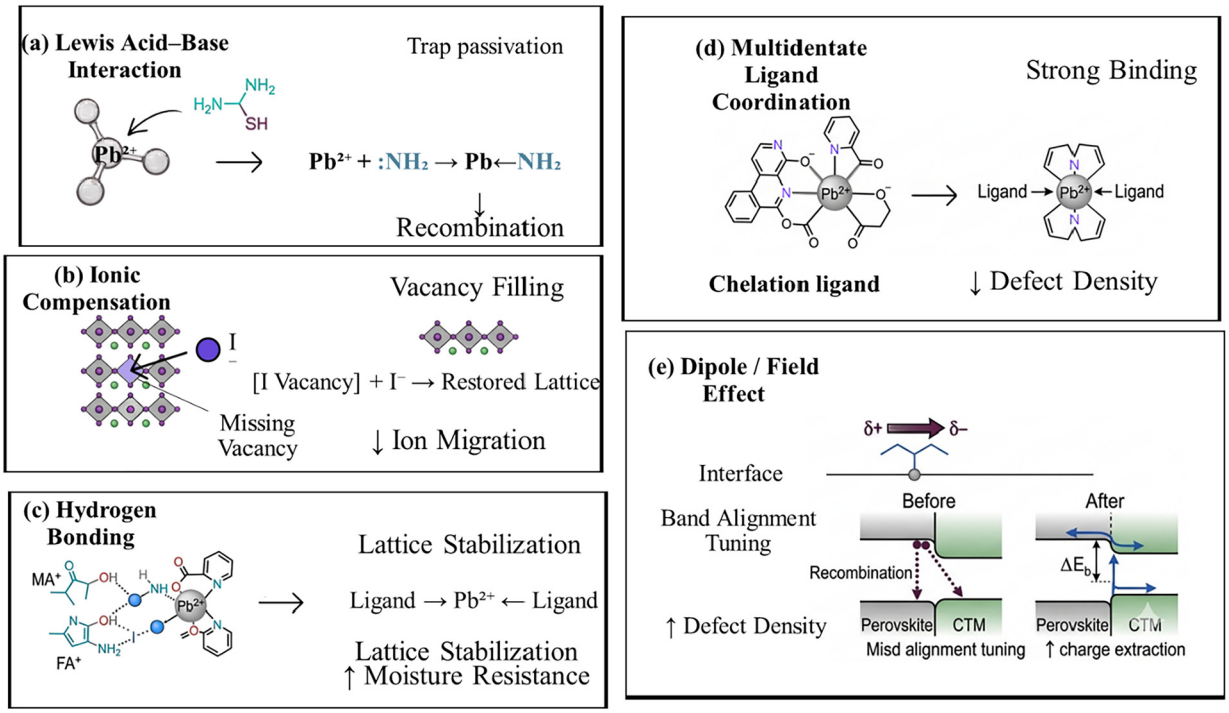

Figure 3. Overview of the molecular mechanisms of interfacial defect passivation, including (a) Lewis acid-base interaction, (b) ionic compensation, (c) hydrogen bonding, (d) multidentate ligand coordination, and (e) dipole-induced field effects, and their roles in enhancing photovoltaic performance

3.4. Coordination Chemistry. Beyond simple Lewis acid-base interactions, coordination chemistry provides a more comprehensive approach to interfacial defect passivation through the formation of well-defined metal-ligand complexes. This strategy involves the strong binding of multidentate ligands or chelating agents to undercoordinated metal centers. Such coordination reduces trap density and enhances chemical stability by suppressing further reactions at the interface. For instance, carboxylate, phosphonate, and pyridine ligands can form strong coordination complexes with Pb^{2+}, thereby improving device efficiency and increasing lifetime [11,22]. However, as with Lewis base passivation, excessively strong coordination can introduce insulating barriers that impede charge transport. Consequently, recent studies have focused on developing ligands with controlled binding strengths and electronic coupling to simultaneously enable effective passivation and efficient charge transfer. In addition to direct chemical coordination, interfacial properties can be modulated electrostatically. Interfacial dipoles can contribute to passivation by modulating energy-level alignment and charge transport.

3.5. Dipole/Field-Effect Passivation. One approach to interface engineering involves incorporating molecules with intrinsic dipole moments to passivate interfaces by modifying the local electric field and band alignment. This method relies primarily on electrostatic bonding and is commonly combined with chemical bonding strategies. Dipole layers can reduce band offsets at the interface, thereby facilitating charge extraction. This can increase the fill factor and reduce recombination losses. Furthermore, the electric field generated by the dipole can promote charge carrier separation in defect-rich regions, thereby decreasing the probability of recombination [23,24]. Of particular interest is the simultaneous control of the electronic structure and defect passivation offered by dipole engineering, which makes it a promising approach for optimizing device performance. However, achieving uniform and stable dipole alignment remains challenging, particularly in large-area devices.

Overall, various passivation strategies offer distinct advantages and limitations. Lewis acid–base coordination and coordination chemistry have proven effective for passivating Pb^{2+}-related defects and can be carefully controlled to avoid compromising charge transport. Ionic compensation effectively reduces halide vacancies and ion migration; however, excessive ionic incorporation may adversely affect phase stability. Hydrogen bonding primarily improves structural integrity and moisture resistance but provides relatively weak defect passivation. Although dipole engineering enhances energy-level alignment and charge extraction, maintaining stable dipole orientation remains challenging. Therefore, multifunctional approaches that combine complementary passivation mechanisms are increasingly promising for simultaneously improving device efficiency, stability long-term performance .

4. INTERFACE TYPES AND THEIR CHEMICAL CHARACTERISTICS

The defect and chemical composition of PSCs are strongly interface-sensitive. Different interfaces exhibit distinct chemical environments, energetics, and defect-formation mechanisms. Therefore, defect-passivation strategies must be tailored to the specific chemistry and charge-transport requirements of each interface. Understanding these differences is crucial for the rational optimization of devices because in many cases, interfacial effects are controlled by local chemical interactions rather than by bulk effects [1,24].

4.1. Perovskite/ETL Interface. The perovskite/ETL interface plays a key role in electron extraction and transport, and its behavior is closely related to defect states and energy-level alignment at the interface. These interfaces are commonly characterized by chemical interactions between the perovskite surface and metal oxide ETLs such as TiO_2 or SnO_2. These interactions may lead to the formation of surface states and trap sites associated with hydroxyl groups, oxygen vacancies, or lattice mismatch. A key issue at this interface is the presence of uncoordinated Pb^{2+} ions and oxygen-related defects, which can create electron-trapping states that hinder efficient charge extraction. Such traps may capture electrons before their transfer to the ETL, thereby increasing the recombination losses and reducing device efficiency. In addition, poor alignment of the perovskite conduction band and the ETL can introduce an energy barrier that further limits the electron-transfer kinetics [15,30]. The interaction between the perovskite and ETL layer is not purely physical interaction but also involves interfacial chemical reactions, including bond formation between the two materials, which may have stabilizing or destabilizing effects. For example, oxygen vacancies or excess hydroxylation on metal oxide surfaces may act as sources of electron traps, and a high density of such traps under humid conditions may lead to degradation. These findings demonstrate that optimizing electron extraction requires consideration of interfacial chemistry, in addition to morphological control.

4.2. Perovskite/HTL Interface. In contrast to perovskite/ETL interfaces, perovskite/HTL interfaces govern hole extraction and transport and are generally more susceptible to chemical instability. Common HTLs include Spiro-OMeTAD, PTAA (poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine]), or inorganic materials, which trigger distinct chemical interactions with the perovskite surface, particularly with organic cations and halide ions. A significant concern at this interface is the occurrence of interfacial reactions between the perovskite and HTL additives, including dopants such as Li-TFSI. These reactions may lead to the formation of new defect states, phase segregation, or even decomposition of the perovskite structure [7,31]. Furthermore, ions, particularly mobile halide ions, may accumulate locally at the HTL interface, altering the local electric field and reducing charge-extraction efficiency. Chemically, this interface is more dynamic than the ETL interface because interfacial reactions and ion redistribution can occur under operating conditions. This dynamic behavior may contribute to the faster degradation associated with the HTL side. Moreover, poor energy-level alignment at this interface may increase recombination losses by creating energy barriers to hole extraction. Thus, the effective passivation of the HTL interface must address chemical stability, defect passivation, and energy-level alignment, making it one of the most complex interfaces to optimize.

4.3. Buried Interfaces. Buried interfaces, which are formed during the sequential deposition of layers in the device

Table 1. *Different chemical passivation mechanisms and their impact on interfacial defects in PSC devices*

Passivation strategy	Chemical interaction	Defect type	Impact on device performance	Limitations	Ref.
Lewis acid–base coordination	Lone-pair electron donation to Pb^{2+}	Undercoordinated Pb^{2+} ions	Reduces trap-assisted recombination and improves V_{oc}	Excessive binding may hinder charge transfer	10,17
Ionic compensation	Vacancy filling and stoichiometric restoration	Halide vacancies	Suppresses ion migration and hysteresis	Risk of phase segregation	18,19
Hydrogen bonding	Hydrogen-bonding stabilization	Organic cation deficiencies	Enhances moisture stability and lattice integrity	Relatively weak interactions	...20,22
Coordination chemistry	Chelation with multidentate ligands	Pb-related defect clusters	Lowers trap density and improves stability	Possible formation of insulating interfacial layers	25
Dipole-field passivation	Dipole-induced electrostatic modulation	Interfacial energy mismatch	Improves band alignment and carrier extraction	Dipole instability over time	24
2D/3D interface engineering	Combined coordination and physical passivation	Surface and buried defects	Improves operational stability and PCE	Thick layers may hinder charge transport	26
Polymer-based passivation	Coordination and electrostatic interactions	Mixed interfacial defects	Suppresses recombination and moisture ingress	Reduced conductivity	27–29
Self-assembled monolayers (SAMs)	Surface dipole tuning	Surface trap states	Enhances charge selectivity and fill factor	Complex fabrication optimization	30
Halide salt treatment	Ionic replenishment	I^-/Br^- vacancies	Improves carrier lifetime and stability	Non-uniform ion distribution	9
Multifunctional organic molecules	Coordination and hydrogen bonding	Multiple interfacial defects	Simultaneously improves efficiency and stability	Molecular design complexity	3
Sulfonyl-based passivation	Synergistic coordination and hydrogen bonding	Pb^{2+} and halide defects	Reduces non-radiative losses	Uncertain long-term durability	22
Amphiphilic polymer additives	Interfacial electrostatic interactions	Grain boundary/interfacial defects	Suppresses charge recombination	Processing sensitivity	28

stack, are increasingly becoming recognized as some of the most critical yet least understood regions in PSCs. In contrast to exposed surfaces, these interfaces are not directly accessible using conventional characterization methods, making their chemical and electronic properties challenging to probe experimentally[2]. Despite this limitation, recent experiments indicate that buried interfaces tend to exhibit high defect densities and substantial recombination losses, primarily because of incomplete crystallization, interfacial strain, and the presence of precursor species. These interfaces can trap charge carriers and serve as recombination centers that cannot be readily mitigated using post-treatment methods. These observations indicate that buried interfaces must be considered beyond simply evaluating defect density. Because of their special chemical environments and their limited accessibility, the molecular interactions governing defect formation, evolution, and passivation must also be understood. Therefore, understanding the chemical nature of buried interfaces and its implications for device stability will be discussed.

From a chemical perspective, buried interfaces are characterized by non-equilibrium states, with defects kinetically trapped during interface formation. Long-term instability can also arise from interfacial reactions between layers, including ion diffusion and chemical incompatibility between materials. In particular, ion migrations toward buried interfaces can lead to charge accumulation and distortion of the local electric field, further accelerating degradation processes[5,32]. The limited accessibility of these interfaces also makes them difficult to investigate, hindering the development of targeted passivation strategies. Post-deposition surface treatments are generally ineffective for passivating buried-interfaces. Instead, passivation must be incorporated during device fabrication through careful control of crystallization kinetics and interfacial chemistry.

Overall, these findings highlight the importance of controlling the film formation and interfacial chemistry during device processing to enable effective buried-interface engineering. Buried interfaces therefore remain among the most crucial, yet least understood, aspects of PSCs, warranting further investigation to

enable the development of highly efficient and stable devices. Further studies must move beyond surface-oriented analyses to improve our understanding of buried interface chemistry. Addressing these knowledge gaps is crucial for improving device performance and achieving laboratory-scale efficiencies under real-world operating conditions..

5. ADVANCED CHEMICAL PASSIVATION STRATEGIES

Recent advances in PSCs have increasingly focused on chemically designed passivation strategies that target interfacial defects through well-defined molecular interactions rather than empirical surface treatments. Functional organic molecules are particularly useful because of their structural tunability and the ability to introduce specific functional groups that interact with defect sites. Undercoordinated Pb^{2+} ions are effectively passivated by electron-donating functional groups, such as amines (-NH_2), thiols (-SH), and carboxylates (-COOH), through Lewis acid-base interactions, thereby improving the electronic properties of the interface. Similarly, polar groups can form hydrogen bonds with the halide ions or with organic cations, thereby stabilizing the lattice. However, although stronger binding can enhance passivation efficiency, excessive molecular coverage or insulating molecular backbones may impede charge transport. Thus, optimum performance requires a balance between chemical passivation and electronic coupling [15,33].

Another promising strategy is the development of two-dimensional (2D)/three-dimensional (3D) hybrid structures in which a thin 2D perovskite layer is deposited at the interface. These 2D layers, typically prepared using bulky organic cations, provide both chemical and physical passivation. Functional groups in the 2D layer interact chemically with surface defects through coordination and hydrogen bonding, and structurally, the 2D layer of the layered architecture provides a barrier against moisture ingress and ion migration. This dual functionality substantially enhances device stability. However, the relative insulating nature of 2D materials may impede charge transport if the layer becomes excessively thick, making precise control of layer thickness and composition crucial [26]. Another promising approach involves polymer-based passivation using macromolecules with multiple functional groups capable of interacting with perovskite surfaces. Conformal polymer coatings, including polyethyleneimine or poly(methyl methacrylate), can passivate defects through coordination, hydrogen bonding and electrostatic interactions while also providing environmental protection. Their scalability and ability to uniformly cover large areas make them attractive for practical applications. However, like other organic layers, polymers may introduce insulating barriers that hinder charge extraction; therefore, their thickness and electronic properties must be carefully optimized [27–29].

Overall, these advanced passivation strategies reflect a shift toward molecular-scale interface design, in which functional groups, interaction mechanisms, and structural properties are carefully engineered to simultaneous achieve defect passivation, efficient charge transport, and enhanced stability. The most effective systems often combine multiple mechanisms, such as coordination bonding and dipole effects, while maintaining favorable electronic properties, highlighting the importance of rational chemical design in next-generation PSCs. The advanced passivation strategies demonstrate that interfacial defects can be suppressed while charge-transfer characteristics and interfacial energetics are simultaneously modulated at the molecular level. Because these chemical interactions ultimately influence the photovoltaic properties of PSCs, understanding their effects on key device parameters is essential, as discussed in the following section.

6. CORRELATION BETWEEN INTERFACE CHEMISTRY AND DEVICE PERFORMANCE

The chemical nature of PSC interfaces, defect states, interfacial energetics, and charge-transport processes is closely interrelated. Rather than acting independently, these factors collectively determine key photovoltaic parameters, i.e., V_{oc}, J_{sc}, fill factor, and overall PCE. Understanding these correlations is therefore essential for translating insights on interfacial chemistry into device-level optimization (Figure 4 and Table 2).

Building on the passivation mechanisms discussed above, changes in interface chemistry directly influence the key photovoltaic parameters of PSCs. Effective chemical passivation, particularly through Lewis acid–base interactions, can significantly reduce the trap density, which is associated with an increase in V_{oc} and PCE [17,34]. Even relatively small changes in interfacial defect density can result in substantial improvements in efficiency, demonstrating the sensitivity of device performance to interface chemistry. Interfacial defects play an important in determining recombination pathways in PSCs, and their presence and distribution depend on interfaces composition. At interfaces with high defect densities, Shockley-Read-Hall (SRH) recombination can dominate, whereby charge carriers occupy the defect states and recombine non-radiatively [35]. These trap-assisted recombination pathways can be suppressed through chemical passivation, thereby promoting radiative recombination. However, complete passivation is difficult to achieve, and residual defects can create localized recombination sites, highlighting the need for uniform interface modification [10,36].

Interface chemistry also plays a decisive role in charge-transport dynamics. Efficient carrier extraction requires appropriate band alignment between the perovskite and charge-transport layers. Interfacial energy levels can be modified through chemical strategies such as dipole engineering and the use of self-assembled monolayers (SAMs), which can lower the energy barriers and facilitate directional charge transfer. In contrast, poorly designed passivation layers, particularly insulating layers, may reduce carrier mobility despite decreasing defects density. This interplay highlights the trade-off between effective defects passivation and electronic coupling, both of which must be optimized to achieve optimal device performance [24,37].

Interface chemistry plays an important role not only in device efficiency but also in stability. Interfacial defects are potential sources of degradation, including moisture-induced degradation, ion migration and phase separation. For example, halide vacancies facilitate ion migration under an electric field, leading to hysteresis and long-term instability. These degradation pathways can be greatly suppressed by chemical passivation strategies that immobilize ions and stabilize the lattice, such as 2D/3D hybrid

structures and hydrogen-bonding networks[7,32]. However, some passivation strategies designed to improve initial efficiency can lead to the formation of chemically unstable species or weak bonds that dissociate over time[38]. This highlights the need to evaluate passivation strategies not only in terms of short-term performance but also under realistic operation conditions. Overall, optimizing interface chemistry and device performance is a multiparameter problem that requires the simultaneous optimization of defect passivation, charge transport, and stability. Integrating complementary passivation mechanisms therefore provides a balanced approach to optimizing defect suppression, charge transport, and long-term device stability.

In conclusion, the efficiency and operational stability of perovskite solar cells are strongly governed by interface chemistry, which influences defect density, charge-carrier dynamics, and interfacial energy alignment. Rational molecular-level strategies can simultaneously suppress non-radiative recombination, facilitate efficient charge extraction, and mitigate degradation pathways. These relationships highlight the importance of chemically controlled interface engineering for the development of efficient and stable PSCs while also identifying the remaining challenges associated with their practical application.

7. CHALLENGES, RESEARCH GAPS, AND FUTURE PERSPECTIVES

Although significant progress has been made in the area of interfacial defect passivation, PSCs still face fundamental challenges that hinder the translation of laboratory-scale efficiencies into stable, commercially viable technologies. One key challenge is the lack of a generalized passivation strategy that can simultaneously address the diverse defect types and interfacial conditions found in PSC architectures. Most current methods are highly system-dependent and are typically optimized to specific combinations of materials and device architecture. Consequently, strategies that are effective at one interface (e.g., perovskite/ETL) may not necessarily be applicable to another (e.g., perovskite/HTL), underscoring the need for a more generalized, chemistry-driven structure[1,24,40].

Another major challenge is the trade-off between defect passivation and charge transport. Trap densities can be effectively reduced through strong chemical interactions, such as coordination bonding or polymer encapsulation; however, these approaches may introduce insulating barriers at the interface that hinder carrier extraction. This trade-off highlights the difficulty of designing interfaces that are both chemically stable and electronically conductive. Existing approaches are often focused on short-term efficiency and may not adequately balance defect passivation with efficient charge transport, resulting in sub-optimal device performance under realistic operating conditions[3,37].

Another important research gap is the lack of data on long-term stability under operating conditions. Most of studies have reported improvements in initial device performance, whereas relatively few have systematically evaluated device stability over extended periods (e.g., 1000–10,000 h) under combined stress factors such as heat, illumination, and humidity. This limitation is particularly significant because interfacial degradation is a dynamic process involving ion migration, chemical reactions, and structural changes. Without large-scale, long-term studies, it remains difficult to assess the effectiveness of passivation strategies[7,41].

One of the most significant unresolved challenges is the limited understanding of buried-interface chemistry. These interfaces form during layer deposition and tend to exhibit high defect densities and experience complex chemical reactions that cannot be readily characterized using conventional techniques. Consequently, much of the current understanding of buried interfaces is derived indirectly, resulting in incomplete or inconsistent models of defect behavior. Addressing this knowledge gap will require the development of advanced characterization techniques capable of probing buried interfaces with high spatial and chemical resolution[2,42].

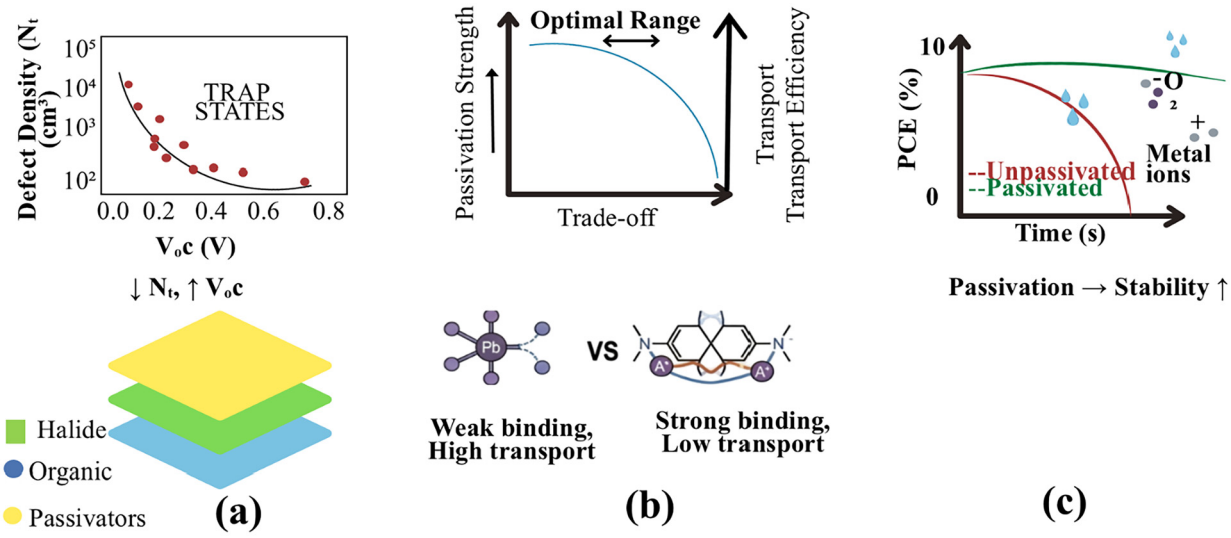

Figure 4. Relationship between (a) interface chemistry, (b) defect passivation, and (c) device performance, illustrating how molecular-level interfacial interactions facilitate charge transfer and reduce defect density and recombination losses, thereby helping enhance device efficiency and operational stability

Table 2. *Correlation between interface types, major defect species, passivation strategy, and photovoltaic performance in PSC devices*

Interface type	Defect species	Passivation strategy	Impact on photovoltaic parameters	Stability improvement	Ref.
Perovskite/ETL	Undercoordinated Pb^{2+}	Lewis base passivation	Increases V_{oc} and FF	Reduces electron recombination	15,30
Perovskite/ETL	Oxygen vacancies	SAM/dipole engineering	Improves charge extraction and J_{sc}	Enhances interface stability	24
Perovskite/HTL	Halide accumulation	Ionic compensation	Reduces hysteresis and improved FF	Suppresses ion migration	37
Perovskite/HTL	HTL additive-induced defects	Coordination chemistry	Improves V_{oc} and reduces recombination	Improves thermal stability	31
Buried interfaces	Defect clusters	2D/3D interface engineering	Enhances PCE and charge transport	Improves long-term stability	2,4
Buried interfaces	Ion accumulation	Polymer passivation	Stabilizes J_{sc} and FF	Improves moisture resistance	29
Flexible PSC interfaces	Mechanical defects	Hydrogen-bond networks	Maintains efficiency under stress	Improves mechanical robustness	29
Metal oxide ETL interfaces	Surface hydroxyl defects	Surface chemical modification	Reduces interfacial recombination	Improves humidity resistance	6
HTL/perovskite interfaces	Dopant-induced defects	Multifunctional molecules	Enhances hole extraction	Reduces chemical degradation	3
Grain boundary interfaces	Mixed ionic defects	Polymer additive engineering	Increases carrier lifetime	Reduces defect evolution	28
Inverted PSC interfaces	Dynamic interfacial defects	Molecular interface passivation	Improves V_{oc} and reduces energy losses	Enhances operational durability	13
Lead-free PSC interfaces	High-density intrinsic defects	Coordination passivation	Improves charge transport	Stabilizes crystal structure	14,39

Looking ahead, several emerging research directions offer promising approaches to addressing these challenges. The integration of artificial intelligence (AI) and machine learning (ML) into the design of passivation materials represents a potentially transformative approach[43]. AI-based models can facilitate the identification of optimal functional groups and prediction of interaction mechanisms, thereby accelerating the discovery of effective passivation agents. This approach represents a shift from empirical experimentation towards data-driven molecular design. Simultaneously, the development of "in situ" and operando spectroscopy techniques could provide important insights into the dynamic nature of interfacial defects. Techniques such as in situ photoluminescence spectroscopy, X-ray photoelectron spectroscopy, scanning electron microscopy, atomically-resolved scanning microscopy, and time-resolved spectroscopy can provide real-time information on defect formation, passivation mechanisms, and degradation process under operating conditions[43–45]. These techniques are critical for establishing direct relationships between interfacial chemical reactions and device performance. Another significant future direction, driven by environmental and toxicity concerns, is the development of lead-free perovskites. However, these materials generally exhibit higher defect densities and lower intrinsic stability, making interface passivation even more critical. A deeper understanding of the distinct chemistry of lead-free systems will also be required for their successful implementation[39]. Finally, scalable and reproducible fabrication remains a critical challenge for commercialization. Many passivation strategies demonstrated at the laboratory scale require complex processing methods or materials that are not readily available for large-scale fabrication. Future research should therefore focus on developing scalable, cost-effective, and robust passivation methods that are compatible with diverse device architectures and fabrication processes. Overall, although substantial progress has been made in understanding and controlling interfacial defect passivation, the field still requires a more cohesive and chemically driven approach. Understanding the interplay among defect chemistry, charge transport, and stability, particularly at buried interfaces, will be critical to realizing the full potential of PSC technology.

8. CONCLUSIONS

As shown in this review, the chemical nature of PSC interfaces fundamentally dictates device performance and stability, with defect states actively influencing charge recombination, ion migration, and interfacial energetics. Interfacial defects, particularly undercoordinated Pb^{2+} ions and halide vacancies, are not passive imperfections but dynamic entities that impose limits on device efficiency and contribute to degradation mechanisms. Therefore, rational chemical design is more effective

than material selection alone for interfacial passivation. Through examination of key interaction parameters, including Lewis acid–base coordination, ionic compensation, hydrogen bonding, and dipole-induced effects, this review highlights that successful strategies must reduce the defect density while maintaining efficient charge transport and enhancing stability. More importantly, passivation strategies can be universally applied, as each interface presents distinct chemical and electronic challenges, with buried interfaces remaining particularly a critical yet understudied region. Progress in this direction requires an integrated, chemistry-based design approach supported by advanced characterization and material-discovery techniques. The scalability and stability of PSCs will depend on balancing passivation with electronic functionality, ultimately helping to bridge the gap between laboratory performance and real-world operation through rational interface engineering. The commercialization of perovskite solar cells will require highly effective passivation strategies that are both scalable and cost-effective. Among the approaches discussed in this review, those based on polymer-based passivation, SAMs, and multifunctional organic molecules are particularly promising because they are compatible with solution processing and large-area coating methods and do not affect the devices efficiency and stability. The development of chemically robust, environmentally stable, and industrially scalable interface-engineering strategies will be a key step in translating laboratory-scale demonstrations into commercial photovoltaic production. Future progress toward PSC commercialization will depend on advances in molecular-level interface engineering, scalable fabrication processes, and long-term operational stability. Combining chemically rational passivation strategies with manufacturing-compatible processes will be essential for translating laboratory-scale efficiencies into reliable and cost-effective photovoltaic technologies at a commercial scale.

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