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Defect Engineering and Carrier Transport Mechanisms in Halide Perovskites for High-Performance Optoelectronic Devices: Recent Advances, Challenges, and Future Perspectives

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ABSTRACT: In recent years, new scientific findings in preparation of perovskite oxides have brought materials with relatively wide band gap to the interest of optoelectronic applications, and the resulted halide perovskites oxide have excellent charge transport (e.g., relatively long diffusion length of carriers), high optical absorption, and are the most promising materials. However, intrinsic/extrinsic defects have a major impact on carrier recombination, ion migration, operational stability as well as device efficiency. In this review, the recent progress on the defect chemistry and the processing (defect engineering) method to control its carrier transport mechanism(s) in halide perovskites is discussed. Key issues such as carrier generation, transport and recombination and the fundamental aspects such as crystal structure, electronic properties, as well as point defects, grain boundary and surface defects, ion migration are critically discussed. The different defect engineering strategies of interface engineering, surface and grain boundary passivation, incorporation of additives, composition/dimensional engineering, quantum dot passivation, and optimization of tin perovskite are systematically examined. Additionally, sophisticated experimental characterization techniques are explained that are coupled with first principles calculation to develop an understanding of the defects and to optimize the device performance. Applications for them are also shown, and current challenges and future opportunities, such as artificial intelligence (AI) tuning of materials and defect Tolerant perovskite design, are discussed. Defect control and carrier transport are closely linked and this review will offer a general view of the link and will benefit the development of various commercially viable highly efficient and stable halide perovskite optoelectronic devices.

KEYWORDS: Halide perovskites; Defect engineering; Carrier transport; Optoelectronic devices; Charge recombination; Ion migration

I. INTRODUCTION

With outstanding optical absorption, tunable band gap, long carrier diffusion length and defect tolerant electronic structure, the halide perovskites has become one of the most revolutionizing materials for modern optoelectronic devices. By using these materials, tremendous strides have been made in photovoltaics, light-emitting diodes (LEDs), photodetectors, lasers and new memories over the last 10 years. One of the most interesting properties is the ease by which halide perovskites can be solution processed and thus be easily integrated in scalable next generation of electronic and photonic devices with this surprising combination of excellent optoelectronic properties. More recently, defect understanding and understanding of carrier transport on the microscopic level – both of which will impact the ultimate device performance, operational stability and commercial feasibility – have become the focus of attention, as have become high efficiencies [1–3].

1.1 Evolution of Halide Perovskites

The general formula of the halide perovskites is the ABX_3 structure, with A being an organic or inorganic monovalent ion such as methylammonium (MA), formamidinium (FA) and cesium (Cs), B typically a divalent metal ion such as Pb^{2+} and Sn^{2+} and X typically a halide ion such as Cl^- , Br^- and I^- . Depending on temperature, and composition, there can be orthorhombic, tetragonal and cubic phases to their crystal lattice which enable for large compositional engineering for specific applications. Although, fully inorganic composition solar cells are thermally stable, such solar cells made from organic–inorganic hybrid perovskites have achieved very good PV efficiencies due to their light absorption capability and moderate transport of free electron and hole. In addition, the awareness to the toxicity of lead

has increased since the rise of the environment awareness and the research of an alternative to lead has taken more momentum, such as the tin-based perovskites and other Perovskite-structured materials, but there are still efficiency and stability to overcome [1,4,8].

1.2 Importance of Defect Engineering

Despite the fact that halide perovskites have excellent intrinsic properties, they are not defect-free but have above-mentioned point defects, grain boundary defects, surface defect states, and interfacial trap states, which have a large role in the dynamics of charge carriers. Defects can either serve as shallow non-destructive states or as deep traps which can kill devices, exercise control on the non-radiative recombination and lifetime, ion migration and device degradation. Hence, defect engineering has become an essential strategy to improve the conversion efficiency, stability, lifetime and scalability of Perovskites opto-electronic devices. However, a growing body of recent research has revealed a rational passivation and interface modification, compositions and dimensionalities optimisation, and enhancement of carrier extraction and environmental durability in the last decades to be effective at suppressing this trap-assisted recombination [2-4].

1.3 Carrier Transport

A second outstanding property of the highly performing halide perovskites is their capability for highly efficient transport of charged carriers. When illuminated, absorbed photons create excitons, which in the materials used typically have a small binding energy between the electron and hole which means that they can easily be separated to create free electrons and holes. The charge carriers have long diffusion lengths and high mobilities, which means that they can be transported efficiently towards the device electrodes before recombining. The defects and the migration of the ions can however affect the transport process by introducing localized trap-states, cause hysteresis and lead to degradation under electric bias or illumination. It is now essential to have interplay between the electronic carriers, excitons and the mobile ions and to obtain the high performance and reliable optoelectronic devices [3,5,7].

1.4 Optoelectronic Applications

However, due to the amazing properties in the electronic and optical field of halide perovskites, a flurry of progress in various optoelectronic technologies has been possible. To achieve the best solar cell efficiency, optimised carrier transport and minimised defect density have resulted in record PVs in solar cells. With efficient radiative recombination and defect passivation, the internal (and external) quantum efficiencies and lifetimes of operation of LEDs can be significantly improved. The same properties (absorption coefficient and band gap that can be controlled) make the materials interesting for application in photodegradation, while a high optical gain is desirable for low-threshold lasers. In recent times, there has been much interest in the resistive switching behavior and ion migration phenomena for novel non-volatile memory and neuromorphic computing applications [2,4,6].

1.5 Scope of the Review

This review critically summarizes all the advancements of defect engineering and the mechanism of carrier transport in the halide perovskites for high-performance optical electronic devices in recent couples of years. The subject of defect chemistry and charge transport processes, passivation strategies, experimental and computational characterization techniques and their combined effect in solar cells, LEDs, photodetectors, lasers and memory devices is given special emphasis. Lastly, the available open questions and future research directions are delved which aim to the aspirations of stable, scalable and commercially viable perovskite technologies.

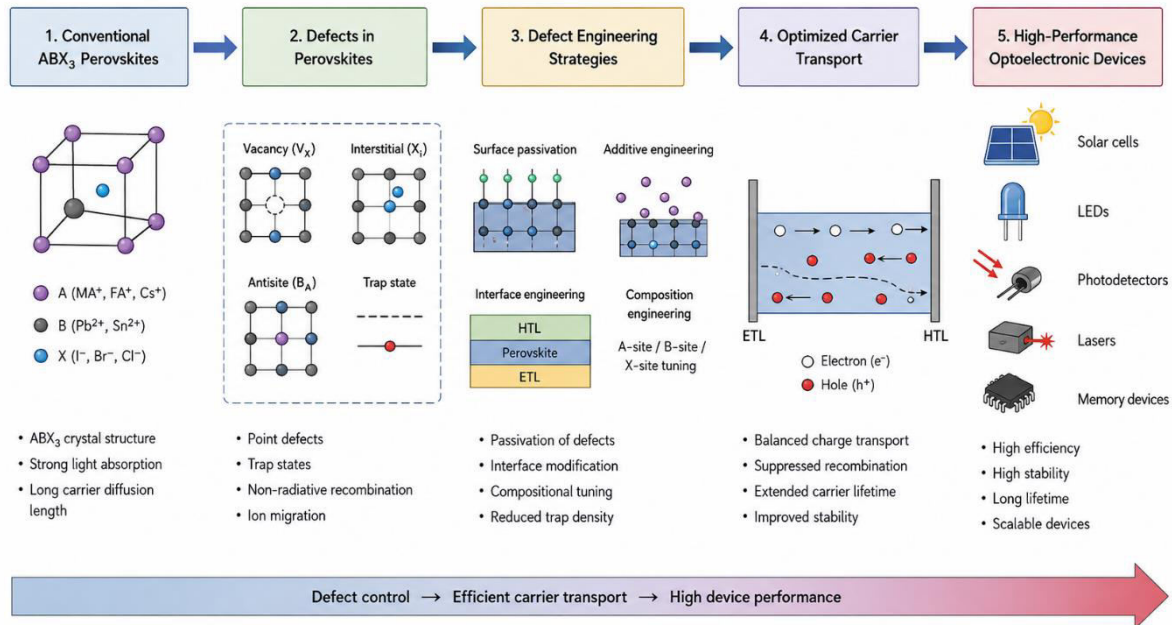


Figure 1. Evolution of defect engineering in halide perovskites.

II. CRYSTAL STRUCTURE AND ELECTRONIC PROPERTIES OF HALIDE PEROVSKITES

The potential of more or less perfect tuning of the crystal structure combined with the remarkable electronic properties of these materials makes the success of halide perovskites in optoelectronic applications remarkable so far. By tuning the composition to achieve precise control of the perovskite lattice, the flexible properties of the bandgap, carrier mobility and optical absorption and defect tolerance can all be optimised and tailored to applications. In contrast with the traditional semiconductors, the lattice of metal halide perovskites is very soft and ionic which avoids the structural distortion but retains superb electronic properties, greatly extending their potential applications in high-performance solar cells, LEDs, photovoltaic devices etc. Knowledge of their crystal symmetry, the electronic band structure, charge generation processes and compositional effects are very important because they will help identifying the main directions for defect engineering to optimize the material performance [9-11].

2.1 Crystal Structure

The crystal structure of halide perovskites is in general expressed as ABX_3 , where A is a monovalent cation (MA^+ , FA^+ , or Cs^+), B is usually a Pb^{2+} or Sn^{2+} , and X is a halide ion (I^- , Br^- , or Cl^-). These can exist in either cubic, tetragonal or orthorhombic configurations depending on the temperature and pressure, and chemical composition. In the cubic phase, there are high crystallographic symmetry and almost ideal octahedral connectivity conditions which make charge transport isotropic. The lower temperature tetragonal and orthorhombic phases, their octahedral tilting and lattice distortion, all affect the band structure and the formation energies of defects and the carrier dynamics. Optimization of the optoelectronic performance and stability of structure under working condition of device is directly linked with the impact of switch of their phases [12-14].

2.2 Electronic Band Structure

Also one of the most interesting features of the halide perovskites is that they have a direct band gap that will allow for efficient absorption of photons and radiative recombination. These valence band states are mostly composed of halide p and metal s and the conduction band mostly of metal p. Consequently, much smaller values of the effective masses of the electron and hole can be achieved that can lead to high carrier mobility and long diffusion lengths. Quite and systematic alterations of the bandgap can be made by subtle compositional modifications thanks to the density of states (DOS) calculations that show that the hybridization and the dispersion of the band structures changes as a function of the composition. It can also be systematically bandgap engineered for optoelectronic purposes due to the density of states (DOS) calculation, the hybridization and the dispersion of the band structures as functions of the composition.

2.3 Charge Generation

The large absorption coefficients over a broad range in the visible spectrum, when illuminated, make halide perovskites highly suited for an efficient absorption of photons. The binding energy of the excitons created is relatively low and excitons rapidly split to free electrons and holes in the ambient temperature. In efficient charge separation (combined with a low trap-assisted recombination rate) the photogenerated carriers are able to diffuse over a micrometer distance to the electrodes. This is an efficient charge generation process that is a key for the excellent performance of perovskite-based photovoltaic (PV) and light-emitting device (LED) [10,11].

2.4 Carrier Lifetime

It is indeed one of the most exceptional characteristics of good halide perovskites that the free carriers exhibit a long lifetime. Due to the low value of non-radiative recombination, and also due to the low effective masses, high values of the carrier mobility and very long diffusion lengths are possible even for well passivated films, often exceeding few micrometers. But, localised trap states can arise because of the structural defects, or because of grain boundaries and compositional heterogeneity, and can affect the lifetime or the transport efficiency. It has been recently shown that the elastically passivated defects help in increasing the average carrier lifetime at the cost of decreasing various recombination pathways and help in electronic uniformity of the perovskite domain by passivating defects [13,17].

2.5 Influence of Composition

The optical and electrochemical properties of the halide perovskites are very sensitive to their chemical composition. For a general trend, the use of formamidinium (FA) in replacement of methylammonium (MA) will help to increase thermal stability, while thought to decrease bandgap and cesium (Cs) will help to increase phase stability and environmental durability. Similarly, the possibility of substitution between the three kinds of anions, iodide (I), bromide (Br) and chloride (Cl), permits the optical absorption and emission wavelengths to be varied continuously by such substitution. Two elements were found to be useful for a high efficiency reference: Lead (Pb) possesses a favorable electronic structure and Tin (Sn) is a potential future replacement of Lead even though there are issues associated with the oxidation, and potential defect sites cannot be created. All of the above advantages can be combined in mixed-cation/mixed-halide compositions, which also have excellent structural stability, optimum carrier transport and high device performance [14,16,18].

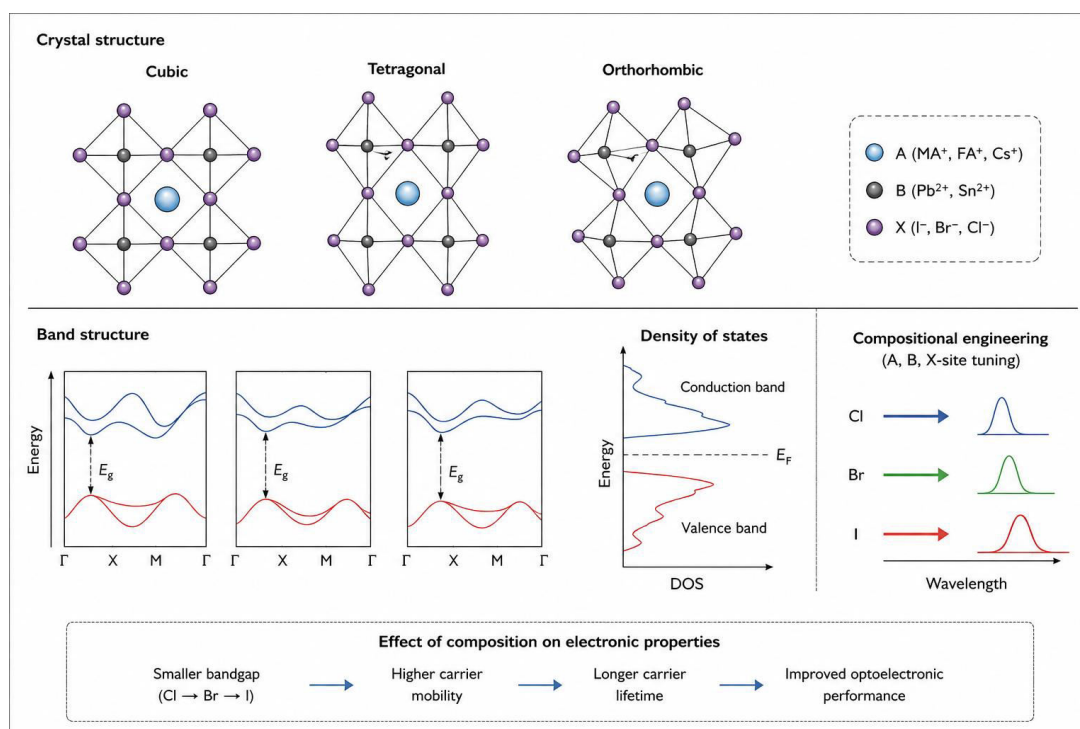


Figure 2. Crystal structures and electronic band diagrams of halide perovskites.

III. DEFECT CHEMISTRY IN HALIDE PEROVSKITES

Defect chemistry is the key factor to understanding the optoelectronic performance, operational stability and long-term reliability for halide perovskites. Unlike conventional semiconductors, (e.g. silicon), halide perovskites possess a rather soft lattice and the defect formation energy is low, so these lattice defects can occur spontaneously and can even move. While much of the defects occurring in these materials have no impact on the electronic functionality as these materials are defect tolerant, others can create trap states that lead to non-radiative recombination, ion migration and degradation of the devices. The knowledge of mechanisms of defect formation and their role in concurrent carrier dynamics is therefore crucial when designing efficient optoelectronic devices based on perovskites. The recently developed experimental characterisation and a series of first principle calculations works have paved important steps towards a deeper understanding of the defect chemistry and the development of effective strategies of defect engineering [19-21].

3.1 Classification of Defects

There are two types of defects in halide perovskites, one intrinsic defects, and one that comes from the environment. Vacancies, interstitials and antisite defects are examples of intrinsic defects which arise during the crystal growth process. Vacancy defect: When atoms are missing from the lattice position interstitial defect: When excess atoms enter into the lattice position. An antisite defect is when one of the lattice atoms is replaced by another of the wrong sort at an appropriate site. Depending on their formation energy and charge state these defects can be shallow traps or deep traps, which change the local electronic structure.

Defects which are purposefully introduced during synthesis and/or unavoidable in the fabrication of the devices, and also through incorporation of foreign species are extrinsic defects. Some impurities may be introduced through precursor materials, solvents and processing conditions and lead to a decrease in crystallinity and an increase in degradation rates, while many may be intentionally added for reasons like improving the concentration of charged carriers, improving the stability of the phases, passivating trap states, etc. Both the type and spatial distribution of intrinsic and extrinsic defects lead to a density of defects that determine the electronic quality of the films and, consequently, the possibility to achieve high performance of perovskite-based devices [20,22].

3.2 Point Defects

Halide perovskites were possibly the most investigated defects being the point defects which have a direct impact on carrier recombination and ion migration. A few typical cases of vacancy defects are iodine vacancies V_I , lead vacancies V_{Pb} and methylammonium vacancies V_{MA} . It is generally found that the formation energy of iodine vacancies is relatively small and that they have a high effect on the ionic conductivity and current-voltage hysteresis. Generally speaking, lead vacancy is able to act as a shallow acceptor and the vacancy of the methylammonium group has a more significant effect on the stability of the lattice and on the ionic transport properties.

Localized electronic states are produced by interstitial defects such as interstitial I_i and interstitial Pb_i which might increase the nonradiative recombination at high defect concentration. They are greatly influenced in their formation by synthesis conditions, synthesis stoichiometry, and environmental exposure. Careful control of composition and defect passivation, as suggested by Density Functional Theory calculations can dramatically decrease these harmful point defects and result in so far excellent carrier lifetimes and device efficiencies [21,23,24].

3.3 Grain Boundary Defects

The majority of the solution processed perovskite halide films are polycrystalline, so that they contain many grain boundaries. Owing to imperfect lattice continuity and less than complete crystal coordination, the interfaces are typically higher in defect density than is the across grain interior. Grain boundaries can trap charge carriers leading to an increase in the recombination of charge carriers and also are prone to migration of ions under an electric field. Grain boundaries also are often a source of diffusional flow of moisture and oxygen, which can act as environmental mitigation factors. Surface passivation and engineering of the grain boundaries has thus proved to be an effective approach resulting in a decrease of the trap density and a better charge transport through the polycrystalline films [22,25].

3.4 Surface Defects

Surface defects play a major role in the imaginary charge extraction at the interfaces in perovskite devices. An electronic state is formed which is also localized by the "under" or "over" coordinated atoms, dangling bonds and

surface vacancies resulting in loss of PV performance and carrier lifetime due to surface recombination. Furthermore, chemically active surface sites lead to reactions with moisture and oxygen, thus to problems concerning the stability in the long term. Increasing yields and operational stability have been obtained with some very recent passivation methods such as the use of organic ligands, Lewis acids, Lewis bases, and low dimensional perovskite layers [23,26] that have proven to be highly effective in rendering the dangling bonds irrelevant and reducing the respective surface trap densities.

3.5 Deep vs Shallow Defects

The effect of defects on the properties of the semiconductor material will be mainly electronic, and depend on the type of energy level that the defects introduce in the band gap of the semiconductor material. Shallow defects produce energy levels near the conduction bands, valence bands and do not, in general, have any significant effect upon the carrier transport since thermally activated carriers are easily released from the defect. In contrast, certain deep defects will create gap states that will be able to easily capture a hole and an electron and will provide an available path for non-radiative recombination. Those deep level defects will lead to the reduction of diffusion length, short carrier lifetime and lower efficiency of the device. Therefore, it is one of the key defect engineering research topics to identify and remove selectively deep trap states [24,27].

3.6 Dynamic Defect Tolerance

But one of the unique characteristics of halide perovskites is their dynamic defect tolerance. A large number of these defects are mobile, with low formation energies, and are very mobile in the soft ionic lattice, and migrate under thermal and/or electrical stimulation. Defect migration plays a role in the hysteresis and degradation, but also provides some self-healing such as relaxation behaviour that leads to recombination or defect migration. Such dynamic behavior is responsible for the remarkable tolerance of the halide perovskites to relatively high defect densities as compared to conventional semiconductors and it is an active research area, both experimental and theoretical [25,28].

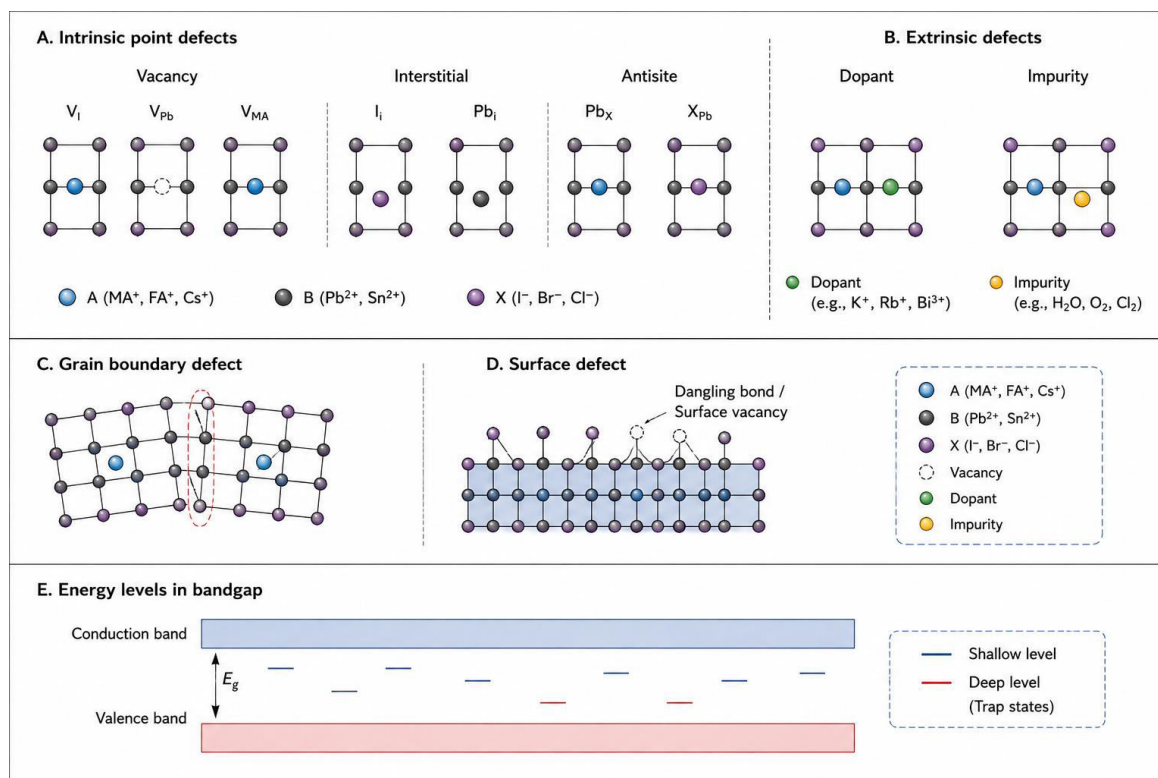


Figure 3. Schematic illustration of intrinsic and extrinsic defects in halide perovskites.

Table 1. Classification of defects in halide perovskites

Defect Category	Defect Type	Representative Examples	Primary Effect on Device Performance
Intrinsic	Vacancy	VI, VPb, VMA	Ion migration, carrier trapping, hysteresis
Intrinsic	Interstitial	Ii, Pbi	Deep trap formation, non-radiative recombination
Intrinsic	Antisite	Pb on halide site, halide on Pb site	Band structure perturbation, localized states
Extrinsic	Dopants	Alkali ions, metal dopants, organic additives	Trap passivation, carrier concentration tuning
Extrinsic	Impurities	Residual solvents, precursor contaminants	Reduced crystallinity, accelerated degradation

IV. CARRIER TRANSPORT MECHANISMS

During this list, one of the emergent features that can influence the exceptional optoelectronic property of the halide perovskites is carrier transport. These unique properties of low exciton binding energy, high dielectric constant and small effective carrier mass facilitate their ability to efficiently generate, separate and transport the photogenerated charge carriers. The intrinsic defects, the grain boundaries, the quality of the interfaces as well as the mobility of the ions however are strong determinants to the efficiency of transport. Hence, understand of basic transport mechanisms becomes very important with the aim of increase of the device efficiency, decrease of the recombination losses and long-term operational stability of perovskite based optoelectronic devices. Recent experimental and theoretical efforts have shed light on charge dynamics, on some of the scattering processes, on the recombination pathways and on the temperature dependent transport properties, which will help to develop effective approaches to improve defect engineering for future technologies based on perovskites [29-31].

4.1 Charge Generation

The charge generation starts with the absorption of the incident photons where electron–hole pairs are generated in the perovskite absorber layer. Due to the high optical absorption coefficient and direct bandgap, the halide perovskite can capture the visible light efficiently and only relatively thin layers are needed. Low exciton binding energy allows exciton spontaneous dissociation to free carriers at the room temperatures and as such fast generation of mobile electrons and holes. The high efficiencies of photon harvesting near the band edge and efficient exciton dissociation (with minimal energy loss) play a prominent role in the remarkable photovoltaic and optoelectronic properties of such materials [29,30].

4.2 Charge Separation

The main issue following carrier generation is that the electrons and holes must be separated efficiently, to avoid their recombination. Built-in electric fields at the interfaces between the perovskite absorber and charge transport layers, in addition to the band alignment between these materials, are mainly responsible for charge separation. However, if the engineering of the interface was correct, the accumulation of carriers might be prevented and this recombination in the interface could be decreased hence increasing the efficiency of carrier extraction. Defect passivation also results in efficient charge separation as less charge carrier can be trapped by grain boundary and interface defects [31,32].

4.3 Drift and Diffusion

In halide perovskites, the transport of the carriers happens via drift and diffusion. Drift transport is controlled by the internal electric field created by the device whereas diffusion is controlled by a carrier concentration gradient created after a photoexcitation beyond the photoexcitation zone. The high mobility and long diffusion length of the charges in halide perovskites can result in the diffusion of photo-generated charges many micrometers before they are

recombined. An improved crystal quality and a reduced defect density result in an improved drift and diffusion transport and hence in an increased charge collection efficiency [32,33].

4.4 Trap-Assisted Transport

Defects that generate localized trap states result in localized disruption of the transportation of carriers as a result of trapping either as an electron or hole. Later, the trapped carriers will recombine via Shockley–Read–Hall (SRH) recombination that is one of the most significant non-radiative loss pathways in perovskite devices. Although shallow traps affect the diffusion length and carrier lifetime not so severely, deep traps can have a strong effect as trapped carriers will stay in the trap for a long mean time to be thermally re-emitted into the conduction or valence bands. The SRH recombination can be suppressed significantly by good defect passivation and the overall transport efficiency improved [30,34].

4.5 Carrier Mobility

The movement of electrons and holes in the perovskite lattice in response to an electric field is given by the carrier mobility. The scattering (mobility) of charge carriers in the good quality crystals is dominated by scattering with lattice vibrations (phonon scattering). Contamination or contamination by impurities, the grain boundaries and other structural defects are other scattering centers which increase the transport resistance, while decreasing the mobility of carriers in polycrystalline films. So, it is extremely important to improve the ratio of crystallinity and the concentration of impurities to get the efficient transport of carriers and better device performances [33,35].

4.6 Recombination Mechanisms

Carrier recombination can take place via radiative, non-radiative and Auger recombination processes. Radiative recombination can create light emissions and this is desirable in the manufacture of LEDs and laser devices. By contrast, non-radiative recombination – also achieved by defect-induced trap states – results in energy being dissipated as heat and in a decrease of device efficiency. At high carrier injection levels, Auger recombination will play more significant a role, which means that instead of a photon being emitted, another carrier is transferred energy from one electron-hole pair that recombines. The processes of non-radiative and Auger recombination continue to play a key role in achieving high performance optoelectronic devices [34,36].

4.7 Ion Migration

Ion migration is one of most appealing subjects of research on halide perovskites since its impact on the stability of the device is secondary; it confirms as a very promising material for photovoltaics. The presence of mobile ionic species such as halides defects, V_I , causes the drift of performances, the accumulation of charges at the interfaces, and the current vs voltage hysteresis, under illumination and at high temperature. The operational instability due to vacancy migration can be understood and this leads to better passivation strategies to effectively suppress migration of vacancies, and to long remaining reliability of the devices [35,37].

4.8 Temperature Effects

The temperature has a significant effect on the carrier transport due to different changes of the lattice vibrations, scattering of carriers, ion mobility as well as phase stability. Raising the temperature will typically increase phonon scattering, ion diffusion and decrease carrier mobility and promote increased defect migration. On the other hand, low temperatures slow down the ionic motion, but can involve structural phase transitions which can change the electronic band structure and the carrier dynamics. So it is critical to understand the transport behaviour as a function of temperature to develop stable-perovskite devices that can be used in a variety of environmental conditions [31,38].

Table 2. *Major carrier transport mechanisms in halide perovskites*

Transport Mechanism	Governing Process	Major Limiting Factors	Influence on Device Performance
Charge generation	Photon absorption and exciton formation	Optical losses	Determines photocurrent generation
Charge separation	Built-in electric field and band alignment	Interface defects	Improves charge extraction efficiency

Drift transport	Electric field-driven carrier motion	Defects, grain boundaries	Faster carrier collection
Diffusion transport	Carrier concentration gradient	Trap density	Controls diffusion length
Trap-assisted transport	SRH recombination via trap states	Deep defects	Reduces carrier lifetime
Ion migration	Vacancy diffusion	Temperature, electric field	Causes hysteresis and instability
Recombination	Radiative, non-radiative, Auger	Trap density, carrier concentration	Determines efficiency and lifetime

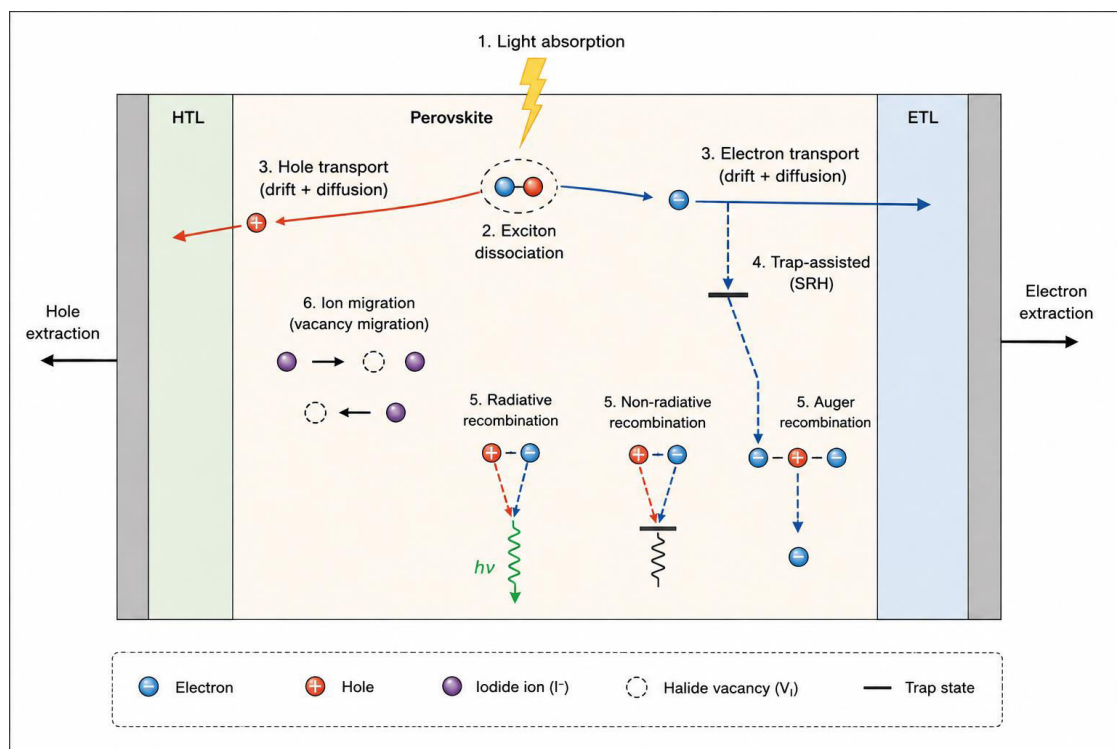


Figure 4. Schematic illustration of carrier transport pathways in halide perovskite optoelectronic devices.

V. DEFECT ENGINEERING STRATEGIES

As one of the most effective approaches, defect engineering has been proven to improve the efficiency, stability and lifetime of the halide perovskite optoelectronic devices. Although the intrinsic defect-tolerant electronic structure of halide perovskites contributes to the lesser impact of the structural defects, structural defects in grain boundaries, surfaces, interfaces and within the crystal lattice introduce trap states that can have a dramatic impact on non-radiative recombination and ion migration processes. Many engineering approaches have thus been exploited to either try to suppress the occurrence of the defect, or to "passivate" any that do occur, while optimising carrier transport. They include interface engineering, surface-passivation, addition of additives, compositional engineering, dimensional engineering and sophisticated computational optimization techniques. All these strategies have contributed significantly to enhancing the performance of perovskite solar cells, LELAMS, photodetectors and others optoelectronic devices [39-41].

5.1 Interface Engineering

An important factor is called the extraction efficiency of the carriers, which is greatly influenced in the presence of interfaces between the perovskite absorber and the charge transport layers. The process of defect passivation allows minimizing the electron buildup at the ETL/perovskite surface and minimizing the interfacial recombination. Similarly, optimizing the hole transport layer (HTL)/perovskite interface helps to minimize the energy barrier and interface trap density and enhance hole extraction. Perovskite devices could be made also much more operationally stable by significantly aligning the energy levels at the surface through application of very thin interfacial layers and self-assembled molecules on the surface [39,42].

5.2 Surface Passivation

One of the defect engineering techniques, which is still widely used, is surface passivation. Organic molecules are also good coordinators for under-coordinated metal ions, and can remove the dangling bonds on the surface of the perovskite material. Small molecular passivators fill-in shallow surface defects and have been demonstrated to greatly reduce the transport of carriers. In addition, Lewis acids could freeze the lone pair electrons of the more electron rich halide vacancies, and Lewis bases could donate pair of electrons to the under-coordinated lead ions. These complementary interactions substantially decrease the surface trap density, the non-radiative recombination and increase the carrier lifetime [40,43].

5.3 Grain Boundary Passivation

There are many interfaces (grain boundaries) in polycrystalline films of perovskite where defects and moisture ('water' more specifically) is known to accumulate. Retrapping of the grain boundary traps and inhibiting the ionic migration can be achieved by using polymer, organic salt and inorganic compound. Simple efficient carrier transport with good environmental stability and good mechanical integrity can be achieved by larger grain size and good passivation of the grain boundaries [41,44].

5.4 Additive Engineering

Additive engineering tunes the crystal nucleation and growth in film formation to obtain high-quality perovskite layers with fewer defects. KI as additives help to effectively compensate the halide vacancies and Rubidium (Rb) enhances the crystallinity and phase stability. However, the effect of hydrogen bonding of guanidinium (GA) and the formation of protective films at the boundary of PEA1 to restrain the interfacial recombination and the moisture induced degradation are further improving the lattice stability. They work as a group to improve the carrier mobility, reduce induced trapping and recombination to extend the lifetime of the carrier in the device [42,45].

5.5 Compositional Engineering

The chemical composition can influence notably the defect chemistry and electronic properties of halide perovskites. Comparing the mixed and single cation compositions, the mixed ones exhibit higher structural stability and lower defect densities than the single ones, if MA, FA and Cs are present in the mixture. Also, a fine tuning of the band gap can be achieved by a judicious carrier transport optimization, in the case of mixed halide perovskites containing iodide, bromide and chloride. Allows to reduce the phase instability and to improve the long term operational performance (compositional engineering) [43,46].

5.6 Dimensional Engineering

Defect suppression by dimensionality reduction of structure has been demonstrated to be an important approach. Carriers in general have good mobility in the traditional 3D perovskites, yet they are not environmentally stable. The more flexible layered crystal structure of 2D perovskites, however, results in excellent moisture stability while mobility of carriers is poor. However, 2D/3D heterostructures are able to overcome the lack of one of these systems, i.e., to create an efficient charge transport along with a high environment stability through effective surface passivation [44,47].

5.7 Quantum Dot Passivation

Surface defects of the perovskite quantum dots are particularly crucial due to its large surface to volume ratio. Surface ligand engineering and surface passivation by an inorganic shell have been shown to be effective tools to successfully reduce the amount of dangling bonds, to suppress the non-radiative recombination and to enhance the photoluminescence quantum yield. Passivation of quantum dots however has been found to be an important method to improve the performance of LEDs, P.O.Ts and display technology [45].

5.8 Defect Passivation in Tin Perovskites

Due to concerns of the toxicity of lead, there has been much interest into making lead-free tin based perovskites. However, some disadvantages are there as Sn^{2+} will quickly be oxidized to Sn^{4+} causing the generation of higher defect densities and hence leading to faster degradation of the device. Although surface passivation by P molecules, oxygen assemblage inhibitor additives and reducing agents have yielded positive results to prevent oxidation, reduce the incidence of vacancy and improve the performance and stability of the tin-based perovskite devices [46,48].

5.9 Machine Learning Guided Defect Optimization

Nowadays, machine learning has become a robust technique, which can speed up the research in defect engineering. This can be achieved using a combination of experimental databases and DFT calculations, in combination with machine learning. This data-driven methodology substantially reduces the computer work and could be used to evaluate defect-tolerant materials with an optimum optoelectronic property. This data-driven methodology can greatly reduce the computational efforts and they can be used to elucidate the defect tolerant materials with optimum optoelectronic property [47,48].

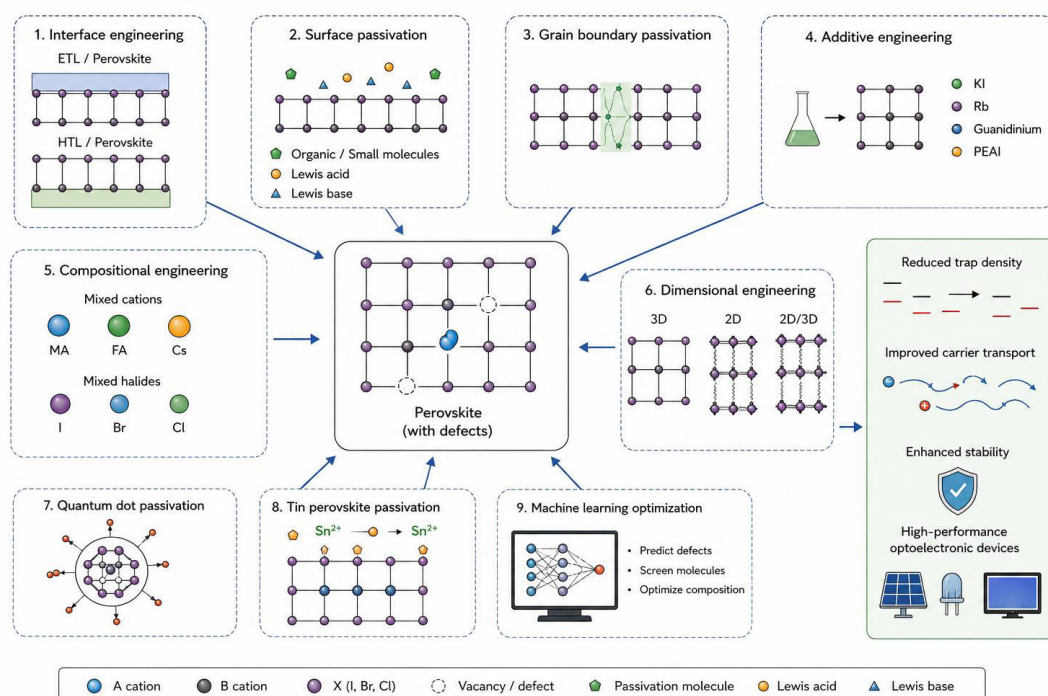


Figure 5. Overview of defect engineering strategies in halide perovskites.

Table 3. Comparison of defect passivation methods

Strategy	Advantages	Limitations	Representative References
Interface engineering	Improved carrier extraction, reduced interface recombination	Requires precise interface control	[39,42]
Surface passivation	Suppresses surface traps and non-radiative recombination	Limited long-term chemical stability of some ligands	[40,43]

Grain boundary passivation	Reduced trap density and moisture penetration	Dependent on film morphology	[41,44]
Additive engineering	Improved crystallinity and defect suppression	Excess additives may alter phase purity	[42,45]
Compositional engineering	Enhanced stability and bandgap tuning	Possible phase segregation in mixed systems	[43,46]
Dimensional engineering	Improved environmental stability	Reduced carrier transport in pure 2D structures	[44,47]
Quantum dot passivation	High photoluminescence efficiency	Surface ligand instability	[45]
Tin perovskite passivation	Reduced Sn oxidation and improved stability	Oxidation remains difficult to eliminate completely	[46,48]
Machine learning optimization	Rapid materials screening and prediction	Requires large, high-quality datasets	[47,48]

VI. EXPERIMENTAL AND COMPUTATIONAL CHARACTERIZATION TECHNIQUES

To understand the defect chemistry and carrier transport in halide perovskites, advanced experimental defect characterization, and defect related computational modeling are required. This can be done by combining experimental and computational methods, where the experimental ones give information directly on the crystal structure and morphology, electronic states and the dynamics of the carriers while the computational ones allow investigation at the atomic scale of the defect formation, electronic structure and transport mechanism of which this is difficult to obtain from the experiment. By bringing the complementary techniques together, this relationship between microscopic defects and macroscopic device performance has helped the development of efficient and stable perovskite optoelectronic devices by leaps and bounds [49–51].

Experimental Characterization Techniques

Typically a structural characterization is performed by X-ray diffraction (XRD) to study the phase purity to obtain the crystal phase, lattice parameters and crystallinity. Analysis of the surface morphology and the lattice arrangement, defects in the crystal and interfaces between the crystal and the film are performed in the SEM and TEM, respectively, concerning the grain size and uniformity of the film. Further experiments of surface roughness and the nanoscopic topography measurements using atomic force microscopy (AFM) have a pronounced impact on influencing the interface charge transport [50, 52].

X-ray photoelectron spectroscopy (XPS) is extensively used to examine the chemical composition and the electronic states of the perovskite materials, which provide the identification of elemental composition, oxidation states and defect related chemical bonding. Optical characterization is primarily performed by the photoluminescence (PL) and the time resolved photoluminescence (TRPL) and provides the information about assessing the radiative recombination, carrier lifetime and associated defects related non-radiative losses. In addition, surface potential and work function on a nanometer scale can be obtained by Kelvin Probe Force Microscopy (KPFM), which can offer a picture of how charge is distributed locally and how the electronic structures are barely different due to defects. Among the various methods available for the study of elemental depth profiles and dopant distribution and ion migration in multilayer perovskite devices, the Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) [49,53,54] is of special interest.

Computational Characterization Techniques

Computational modelling of defect formation, electronic properties and pathways of carrier transport (atomistic understanding). To date, Density Functional Theory (DFT) is the most popular tool to calculate the formation energies of defects, the electronic band structure, density of states and charge density distributions, having many successful

applications. A hybrid DFT method thus helps to reduce this overestimation of the band gap prediction and the GW approximation has the opposite effect of adding one to the other, which helps with the accuracy of the predicted quasiparticle electronic structure in optoelectronic materials, as illustrated in the examples above.

Molecular dynamics (MD) simulations are typically performed to explore dynamic processes such as migration of ions, and thermal stability and structural evolution. At the device level, numerical simulators such as SCAPS are available to qualify the PV performance by simulating carrier transport, carrier recombination, interface characteristics and even the density of defects under various solar PV operation conditions. Further device simulations can be used to gain insight into how charges are extracted, distribution of the electric field, and maximum efficiency [56,57].

Combined Experimental-DFT Studies

Most present studies make a mixture of experiment and first principles calculation to gain a complete understanding of defect behaviour. Experimental methods provide insights into the crystal structure, chemical composition and carrier dynamics, while the DFT calculations give insights into the electronic mechanisms behind the observed phenomena. This type of integrated approach helps to identify defect states accurately, predict the possible passivation mechanism, optimize the interface engineering strategy and rationally design high-performance perovskite materials. Computational modelling and experimental observations have therefore formed a valuable combined tool to further advance and accelerate the development of stable and efficient (halide) perovskite optoelectronic devices [52,58].

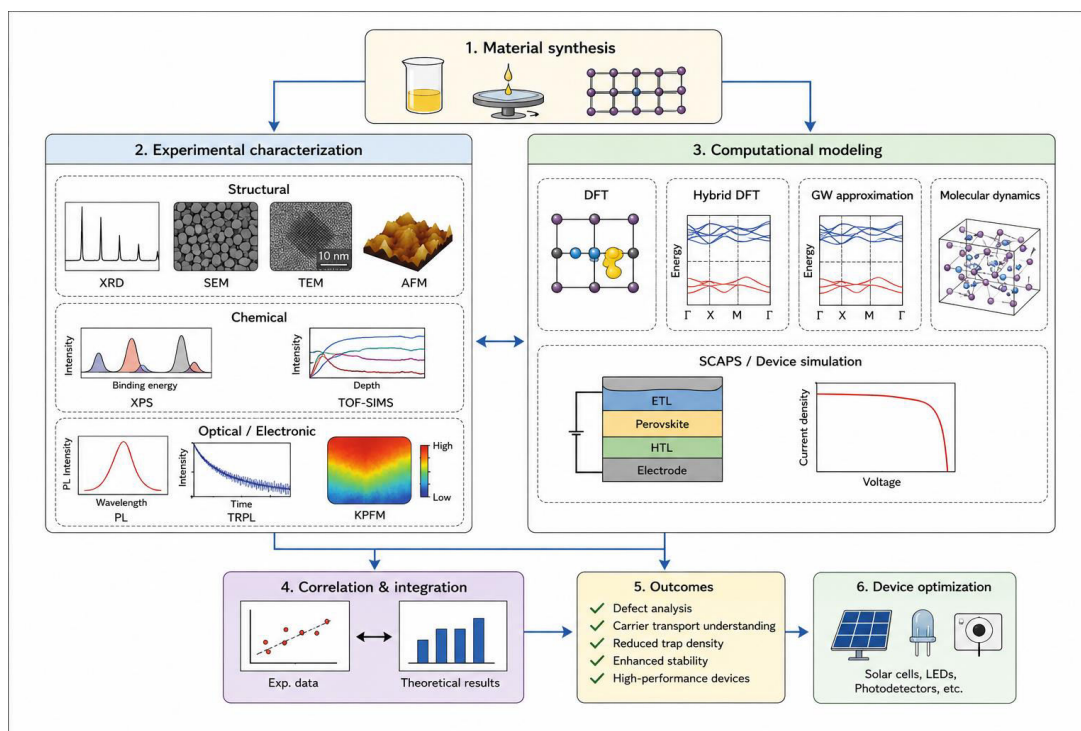


Figure 6. Integrated experimental-computational workflow for halide perovskite characterization.

VII. DEVICE APPLICATIONS

In recent years, halide perovskites have been embraced in various electronic and photonic devices thanks to unprecedented optoelectronic characteristics and recent breakthroughs in defect engineering. A low defect density results in a reduction of loss of carriers due to defect recombination processes, a suppression of migration of these carriers to defects, and a better carrier transport and environmental stability, all of which have a direct influence on the efficiency of the device and its useful life. Defect engineering strategy however will be different depending on the device architecture (e.g. depending on how the charges are transported in the device), wanted charge injection, etc., and depending on the operation of the device. Hence, the modern passivation techniques are crucial to obtain the optimum

performance of PV, LED, photodetectors, lasers, memory devices, and more recently, flexible electronics based on perovskite materials [59-61].

7.1 Solar Cells

The power conversion efficiency (PCE) of perovskite solar cells has been continuously boosted to impressive levels thanks to their properties of favourable light absorption, long diffusion length of photogenerated carriers, and favourable transport of both electrons and holes. Non-radiative recombination suppression and improvement in open circuit voltage and fill factor has been successfully demonstrated by defect reduction via interface passivation, additive engineering and compositional optimization. Meanwhile, essential characteristics such as moisture resistance, thermal stability and durability of the perovskite solar cells are significantly enhanced after passivation processes, making the perovskite solar cell more commercial [59,62].

7.2 Light-Emitting Diodes (LEDs)

Balancing charge carrier injection and radiative recombination in the active layer is difficult and essential to efficiently emit light from a perovskite LED. Surface and interface passivation reduces the trapping losses and boosts the compensation effects of electrons and holes. The strategies of optimized defect engineering have thus been used to boost up the luminescence efficiency, external quantum efficiency (EQE) and to elongate the device lifetime [60,63].

7.3 Photodetectors

The perovskite photodetectors can be with a fast photoresponse and broad spectral response due to large optical absorption and high mobility of the carriers. Defect passivation results in low surface leakage currents, low dark current, consequently in higher S/N and device stability. The collection efficiency of the photogenerated carriers can also be improved in low light conditions because the density of the traps is reduced, which increases responsivity, detectivity and the response speed [61,64].

7.4 Lasers

A perovskite that is a halide would be a great laser gain material because it has a high optical gain, good radiative recombination properties and it is a low threshold laser material. Defect engineering for optical scattering reduction, along with non-radiative recombination reduction leads to a lower lasing threshold, higher optical gain, and more stable emission. Thanks to improved crystal quality and interface control, almost all coherent light generation and operating reliability are further improved [62,65].

7.5 Memory Devices

The fact that halide perovskites are capable of ionic and electronic mixed conductivity has sparked great interest in resistive memory devices. Moreover, controllable defect engineering could enable controllable assertion of resistive switching behaviour based on the migration of vacancies and forming of conductive filaments. Furthermore, tunable ionic transport and dynamic defect behaviour has been hinted to greatly propel neuromorphic computing applications in which devices made up of perovskite materials have been employed to mimic the function of biological synapses, demonstrating a low-power consumption [63,66].

7.6 Emerging Flexible Devices

Halide perovskites are also very promising for applications of wearable electronics and flexible electronics, due to their solution-processability and mechanical flexibility. When defects are passivated, very high carrier mobility is obtained when the material is bent over and over, with simultaneously improved mechanical durability. Together with the ability to be deposited on flexible substrates and to adopt low-temperature manufacturing strategies, defect-engineered perovskites have shown good performance in flexible solar cells, flexible (wearable) photo detectors and (flexible) LEDs as well as integrated multifunctional electronic systems [64,67,68].

Table 4. Device performance after defect engineering

Material	Defect Engineering Strategy	Efficiency / Performance Improvement	Stability Improvement	Reference
MAPbI ₃	Interface passivation	Increased photovoltaic efficiency and reduced recombination	Improved operational stability	[59]
Mixed-cation perovskite	Surface passivation	Higher carrier lifetime and power conversion efficiency	Enhanced moisture resistance	[60]
CsPbBr ₃	Grain boundary engineering	Improved carrier transport and reduced dark current	Better environmental stability	[61]
Hybrid perovskite	Additive engineering (KI, Rb, PEAI)	Reduced trap density and improved charge extraction	Longer device lifetime	[62]
2D/3D perovskite	Dimensional engineering	Enhanced LED luminescence and EQE	Improved thermal stability	[63]
Perovskite photodetector	Surface/interface passivation	Higher responsivity and detectivity	Reduced performance degradation	[64]
Perovskite laser	Crystal defect passivation	Lower lasing threshold and higher optical gain	Improved emission stability	[65]
Tin-based perovskite	Sn defect passivation	Enhanced carrier transport and reduced oxidation	Increased operational lifetime	[66]
Flexible perovskite devices	Interface and compositional engineering	Stable performance under mechanical deformation	Improved flexibility and durability	[67,68]

VIII. CHALLENGES AND FUTURE PERSPECTIVES

In the last decade halide perovskites have drastically progressed in the research but still some scientific and technological challenges remain stop its commercialization. Thanks to defect engineering, the efficiency and stability of these devices has greatly increased however their long term reliability in operational conditions is still a major challenge. Lab-scale optoelectronic innovations will need to be overcome before commercial applications, such as toxicity of the materials, thermal instability, material migration, scalable manufacture, and environmental stability. Meanwhile, new computational methods and state-of-the-art materials design techniques offer valuable opportunities to develop an entirely new generation of defect-tolerant and stable perovskite devices [69-71].

A major drawback of the present halide perovskites is the presence of lead (Pb) which has raised concerns about possible impact on environment and health which has resulted in intensive research efforts for lead-free versions. Among these, there is the family of tin-based perovskite with the same electronic structure, which has received some noteworthy interest. The rapid oxidation of Sn²⁺ into Sn⁴⁺ leads, however, to the creation of the high densities of

vacancies and deep trap states leading to accelerated degradation and less efficient devices. The development of novel stable lead free perovskites with electronic properties similar to the lead based perovskites is therefore key areas of research [69,72].

The migration of ions is a still ongoing challenge, and primarily occurs due to migration of halide vacancies induced by electrical bias, illumination thermal stress. Ion migration is responsible for current–voltage hysteresis, interface charge build-up, phase segregation and degradation of the performances when the devices are considered for long-term operation. Evaporation of moisture and thermal degradation processes associated with ionic migration are capable of driving perovskite to chemical disintegration and changing in structure. Environments stability has been significantly enhanced by encapsulation or passivation/semiconducting materials, however, operation lifetime which is comparable to many silicon technologies is still challenging to achieve (decades) [70,73,74].

But from a manufacturing perspective, there are still large area film depositions, defect uniformities, reproducibilities and process scalabilities, which are limiting industrial implementations. The creation of large substrate size, high-quality crystals and low defect density is much harder for that kind of devices as opposed to the laboratory type devices. Additionally, commercialization would have to involve economically reasonable fabrication techniques, environmental friendly precursor chemistry, long-term stable operation and adherence to ever-tightening regulations regarding the use of toxic materials [71,75].

In the future, Artificial Intelligence (AI) guided materials discovery will be able to revolutionize defect engineering by quickly calculating defect formation energies, and efficiently screen new perovskite materials, and suggest the ideal passivation molecule. Incorporation of machine learning with Danny and high throughput experimentation can drastically speed up the optimization of materials with decrease in computational time and experiments [76].

One of the most prevailing targets is self-healing perovskites, in which the defect “heals” on its own while the perovskite device is in use, when a certain type of motion or “diffusion” occurs among ionic species. Together with ‘interface atomic engineering’, in which interfaces can be modified atomically to reduce the number of trap states at the interface and optimize the band structure, these strategies can make a substantial contribution to the increased efficiency and long-term stability. Meanwhile, compositionally and structurally engineering intrinsically defect-tolerant perovskite might be a significant effort that has not solely been realized through post-synthetic passivation [77,78] to decrease the non-radiative recombination.

Further potential applications are expected to grow with perovskite/silicon tandem photovoltaics that can exploit complementary bandgaps to achieve efficiencies that are greater than the Shockley–Queisser limit and flexible optoelectronic devices such as wearable solar cells, bendable photodetectors, flexible LEDs, and integrated electronic systems. However, still some other concerns remain, and more advanced characterization tools along with more intelligent design of materials, and simulation based on the first principles, will be necessary for the development of commercially viable technology of halide perovskites [79,80].

IX. CONCLUSIONS

Halide Perovskites are one of the most successful material systems developed for next generation optoelectronic devices due to their excellent optical absorption, long carrier diffusion lengths and tunable electronic structure and their exceptional defect tolerance. The fundamental relationship between crystal structure, defect chemistry, carrier transport mechanism and device performance has been summarized and their interaction is emphasized to be important in understanding and addressing problems of device efficiency and stability of perovskite-based devices. Particular efforts have been focussed on gaining insight into the importance of intrinsic and extrinsic defects and their impact on charge transport processes, recombination and ion migration.

Of the many defect engineering methods reported so far, interface engineering, surface and grain boundary passivation, additive engineering, compositional optimization and dimensional engineering have shown the best results to decrease the trap density, suppress non-radiative recombination, increase the carrier mobility and enhance the operational stability. In addition, the knowledge of the behaviour of defects at the microscopic and device scale, achieved by advances in the passivation of quantum dots, tin-based perovskites, and the experimental and computational characterisation of these, has grown considerably.

But, there are important things on which research is still needed. But a lack of long term environmental stability, toxicity of lead, oxidation of tin, ion migration, and scalability of manufacturing have hampered it from going mainstream. Better fundamental knowledge of the behavior of defects in more realistic operating environments, and more reliable models of defect formation and passivation, will be needed to solve these problems. The newly emerging approaches (materials discovery using artificial intelligence, engineering the interfaces at the atomic level, intrinsically defect tolerant materials and tandem-constructed photovoltaics architecture, flexible optoelectronic systems) will be increasingly significant in the future research.

As a whole, ongoing research to combine sophisticated characterization, first-principles computational modeling and rational defect engineering will establish the scientific underpinning for the creation of highly efficient, environmentally stable, and viable halide perovskite optoelectronic devices for a wide array of future energy and electronic applications.

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