**Perovskite Bandgap Tuning to Optimize Light Absorption**

**Material engineering: Developing new perovskite compositions with tailored bandgaps to optimize light absorption**

Miah, H., Khandaker, M.U., Rahman, B. (2024) Band gap tuning of perovskite solar cells for enhancing the efficiency and stability: issues and prospects, RSC Adv., 14, 15876-15906, <https://pubs.rsc.org/en/content/articlehtml/2024/ra/d4ra01640h>

Kulkarni, S.A., Baikie, T., Boix, P.P., et al. (2014) Band-gap tuning of lead halide perovskites using a sequential deposition process. J Mater Chem A., 2, 9221-9225

Tao, L., Qiu, J., Sun, B., et al. (2021) Stability of mixed-halide wide bandgap perovskite solar cells: Strategies and progress, J Energy Chem., 61, 395-415

Bush, K.A. ∙ Frohna, K. ∙ Prasanna, R. (2018) Compositional engineering for efficient wide band gap perovskites with improved stability to photoinduced phase segregation

ACS Energy Lett.; 3:428-435

Saliba, M. ∙ Matsui, T. ∙ Seo, J.-Y. (2016) Cesium-containing triple cation perovskite solar cells: improved stability, reproducibility and high efficiency, Energy Environ. Sci.; 9:1989-1997

*The experimental findings showed power conversion efficiency (due to number of carriers increased) and the short circuit current density increased (due to more photons falling on it); however, the fill factor and open-circuit voltage reduced (due to an increase in dark saturation current) with the increase in the film thickness (*[*Figure 7*](https://www.mdpi.com/2076-3417/13/4/2051#fig_body_display_applsci-13-02051-f007)*). It is noted that more photons were absorbed when the film thickness was increased. These photons could penetrate deeper into the absorber layer, resulting in the production of more electron-hole pairs in devices. The photovoltaic parameters (fill factor = 81.59%, open-circuit voltage = 1.0997 V, power-conversion efficiency = 33.46%, short-circuit current density = 37.17 mA/cm2) were studied under optimized conditions (Ahmad et al., 2022).*

Ahmad, U., Kumar, S., Hassan, A., and Mohsen, M. (2022) High power conversion efficiency of lead free perovskite solar cells: A theoretical investigation. Micromachines, 13, 2201.

The power conversion efficiency reached 22.96% (simulation model) and 8.41% (fabrication model) based on the experimental results.

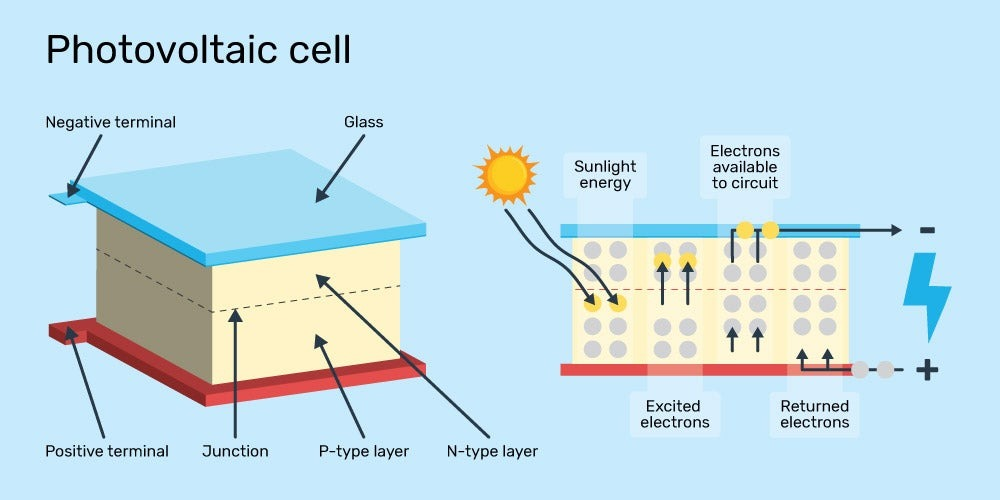
*The photovoltaic behaviors (fill factor = 82.01%, open circuit voltage = 0.95V, power conversion efficiency = 26.33%, short circuit current density = 33.85 mA/cm2) were investigated in specific solar cells (Zn0.75Mg0.25O/CH3NH3SnI3/MASnBr3) (Nihal et al., 2021).*

Nihal, G., Salma, H., Ahmed, S., and Fedawy, M. (2021) Design of lead free perovskite solar cell using Zn1-xMgxO as ETL: SCAPS device simulation. Optik, 242, 167306.

Perovskites can be tuned to various bandgaps within a wide range, while other materials only have one. Perovskite materials can have their composition and structure modulated in order to modify their optical and electronic properties to achieve optimal operating performance. Bandgap tuning, adjusting the range of energy of light that the perovskite materials can absorb efficiently, through structural modification can be used to achieve both high-performance and high-stability PSCs in the presence of extrinsic (moisture, oxygen, UV light, heat, and electric field) and intrinsic (structural and chemical instability, ion migration, and crystal defects) degradation factors (Xia et al., 2023; Xu et al., 2024; Yang et al., 2024). The bandgap should ideally be modified to match the wavelength of solar energy to maximize light absorption. According to Ou et al. (2019) and Miah et al. (2024), methods investigated for band gap engineering and tuning in perovskite materials include compositional engineering or substitution, doping, interface engineering, dimensionality modification, strain and pressure stimuli, and phase segregation and transition. Studies which have adjusted bandgap by various means include: chemical management (Noh et al., 2013), chemical vapor deposition process (Kim et al., 2016B), sequential deposition process for mixed halide perovskites (0 ≤ x ≤ 1)) (Kulkarni et al., 2014), modifying the A cation size (Eperon et al., 2014), pressure engineering (Liu et al., 2019A), and band gap tuning of via substitution of I with Br ions (Tanaka et al., 2003).

All solar cells, including perovskites, create electricity from the photovoltaic effect, which means harvesting energy from the light from the sun. One negative layer and one positive layer of photovoltaic material comprise a solar cell, with conductive electrodes on the front and back to carry the electrons from the sun from the negative layer along a wire to produce electricity before returning them to the positive layer. Electrons float around the nucleus of an atom, with the negatively-charged electrons and positively-charged nucleus attracted to each other. Individual atoms then combine to form molecules based on the number of electrons in each atom, with the shared electrons floating around the molecule. Perovskite solar cells create electricity when photons of light push the outermost, or valence, electrons of a semiconductor material into a higher energy state, from the valence band and into the conduction band of the molecule. The photons of light hit the perovskite absorber layer, exciting and freeing perovskite electrons, creating an electron-hole (e-h) pair. The load is powered via the electron moving towards the HTL, which transports the electron to the conductor. The electrons power the load by flowing as an electric current, then they get collected by the ETL in the perovskite solar panel; the ETL also suppresses the backflow of holes. The perovskite atoms form molecules with other atoms that are semiconductor materials, whose electrons can be excited by light energy and directed along a wire to produce electricity. In a process known as surface recombination, some excited electrons fill holes instead of flowing through the load as electricity, accounting for some of the perovskite solar power losses.[[1]](#footnote-0) The minimum amount of energy needed to push an electron from the valence band to the conduction band is known as the bandgap energy, as electrons in the conduction band no longer orbit the molecule, and instead become a charge carriers that can move through the semiconductor material carrying electrical energy (Zientara, 2025). An encapsulation layer is used to seal solar cells to protect them against damage from weather once mounted in a solar module. Figure 1 shows a photovoltaic cell, and the photoelectric effect. Perovskite solar cells have a special optoelectronic manner, or a tunable bandgap, which is favorable for the efficient conversion of sunlight into electricity. The main absorbing material, or active layer, in a perovskite solar cell, can be either lead halide or tin. In a solar cell, the perovskite absorber, active layer, is attached to other materials layers, such as HTL and ETL, which force electric current to flow in a single direction through the absorber layer and into the metal contacts, electrodes, to be collected as electric current. A thin layer of perovskite absorbs light, which excites charged particles, or electrons, and when these excited electrons are extracted, they generate electric power (Garcia, 2024). In a typical tandem perovskite-silicon device, sunlight interacts with the top perovskite cell first and releases electrons from the perovskite material, leaving behind positively charged holes. The electrons travel into an adjacent charge-collection layer (electron transport layer, ETL), and onwards to an electrode (silver, gold, or copper). Holes migrate in the opposite direction through the hole transport layer (HTL). The silicon bottom cell undergoes the same process, absorbing the lower-energy photons missed by the perovskite cell (Peplow, 2023).

**Figure 1. Photovoltaic Cell**



Zientara, Ben (2025)

<https://www.solarreviews.com/blog/are-perovskite-solar-cells-the-future-of-solar-power>

Halide perovskites possess direct-bandgap semiconductors with a bandgap ranging across the whole visible spectrum (Brenner et al., 2016). Direct-bandgap leads to high photoluminescence yield, and means that the charge carriers in perovskite layers can be efficiently generated in a photovoltaic device or recombined in a light emission device, without any assistance from phonons (Braly et al., 2018). Perovskite bandgap tunability allows for the creation of multicolor light emission devices (Ou et al., 2019). Due to possessing a tunable bandgap, metal halide perovskites exhibit light emissions ranging from ultraviolet to near-infrared wavelength. This range of light emissions is due to both the intrinsic tuning of composition (such as the seamless mixing ratio of halides) in a perovskite, and also because perovskites’ dimensionality can be easily controlled. External stimuli which can affect the bandgap of perovskites include light- or electric field-induced phase segregation (ion migration), phase transition by thermal or moisture, and mechanical effects of strain and pressure (Ou et al., 2019). The position of halides (X) anions in the perovskite crystal structure is most tuneable, though the substitution of the cations (A) and metal (B) can also redefine the bandgap of a perovskite and extend the emission spectrum.

The bandgap of a perovskite crystal is easily tuned simply by changing the mixing ratio of the halides (e.g., I–Br, Br–Cl), or by tuning the halide content and the cations in the perovskite (Liao et al., 2016A; Sutherland and Sargent, 2016), such as increasing the bandgap by increasing the bromine content. The optical band gap derived from the UV-Visible spectrum of the semiconducting material should match the solar spectrum range (1.1–1.5 eV) (Almeida and Maciel, 2018). Varying the halide composition between iodide and bromide in perovskite can tune the bandgap to between 1.55 and 2.3 eV, enabling variation in colour and optimisation for applications in multi-junction solar cells (Noh et al., 2013). The optimum band gap is around 1 eV for the bottom silicon cell in a tandem architecture, meaning that wide band gap perovskite absorbers should be utilized for the top cell (Meillaud et al., 2006). The optimal bandgap for a single-junction solar cell is between 1.1 and 1.4 eV (Meillaud et al., 2006). High-efficiency perovskite-silicon tandem solar cells would have a top perovskite cell bandgap requirement from 1.6 eV - 1.8 eV, and the bottom cell bandgap, such as silicon, of between 0.9–1.2 eV, ideally at 1.12 eV (Tao et al., 2021). Electronvolts (eV) is the unit used to measure the different amounts of energy carried by photons of different colors, with photons of visible light having energies of between 1.75 eV (deep red) and 3.1 eV (violet). Tandem cells work on the theory of spectral splitting, where the solar spectrum is divided by stacking solar cells of different band-gaps on one another, and rely on wide-bandgap (WBG) materials, semiconductors that absorb higher-energy and shorter wavelength (bluer) light, while letting lower-energy and longer wavelength (redder) light pass through to the bottom cell. The top cell needs a wider bandgap to absorb high-energy photons efficiently while being transparent to lower-energy photons. The bottom cell needs a narrower bandgap to absorb the remaining lower-energy photons that the top cell didn't capture. The host material itself may also be modified to create intermediate energy levels or intermediate energy bands to accomplish spectrum splitting. In the case where a single connection or junction between layers of positive and negatively-charged materials undergoes spectrum splitting, the intermediate energy levels or bands give rise to multiple energy gaps suitable for absorbing photons of a wide energy range, and the ideal bandgap conversion rate for these single cells is 33.7% of all incoming light to electricity. The ideal power conversion efficiency of a solar cell, the Shockley–Queisser limit, is the amount of solar energy that can be converted to electricity by a solar cell, correlates to a bandgap of 1.34 eV, because that’s the point at which the maximum amount of visible light will convert electrons to charge carriers (Shockley and Queisser, 1961; Zientara, 2025). The theoretical maximum energy conversion efficiencies for the Shockley–Queisser limit are determined using a detailed balance approach (incoming energy is balanced with outgoing energy), and assuming that each photon above the band-gap gives rise to just one electron-hole pair, while all photons with energy below the band-gap are lost (Solanki and Beaucarne, 2007).

Upon illumination, the perovskite layer generates both excitons and unbound electron–hole (e-h) pairs. The exciton binding energy is sufficiently low for these photogenerated excitons or e-h pairs; thereby it readily undergoes thermal dissociation resulting in free carriers. Combined with high charge carrier diffusion lengths in the μm range and charge selectivity offered by the adjacent ETL and HTL layers, the charges are extracted efficiently at the respective electrodes (Elumalai and Uddin, 2016).

However, no single material we know of has the perfect bandgap to reach the Shockley–Queisser limit. The 1.2 eV theoretical bandgap of silicon solar cells translates into a maximum PCE of around 32%, while the best perovskite materials can reach about 31% PCE. These PCEs are relatively low, mainly because of the thermalisation and transmission losses, which account for about 56 % loss of photon energy, and which result from a single energy bandgap, , being used to convert a wide range of solar energy photons. In this equation, the photon energy is denoted by , or Planck’s constant, and is the frequency of the photon. represents red photons in the solar spectrum which have energy lower than the bandgap energy, and consequently are not absorbed in the material or converted into electricity, and thus represents a transmission loss. Conversely, denotes the high energy photons having energy higher than the bandgap energy, and consequently get absorbed in the material. When the high energy photons are absorbed, the energy difference, , increases the kinetic energy of the electrons, while potential energy rises when a part of the photon energy is used to excite electrons across the band-gap, . Hot electrons possess high kinetic energy, while due to lattice scattering electrons lose their kinetic energy (thermalization) in the form of heat, in a matter of picoseconds. According to Solanki and Beaucarne (2007), in a single junction Si cell, about 33 % of the incident photon energy is used to increase the kinetic energy of the electrons in the conduction band. Hot carrier thermalization loss occurs when the energy difference cannot be converted into electricity and a loss presents. Reducing thermalisation losses in solar cells would result in significant improvements in efficiency. An option to reduce thermalization losses in solar cells is the design of a particular hot carrier solar cell, which are designed to collect electron-hole pairs before they thermalise to, or get cooled to, their respective band edges. Hot carrier solar cells require both an absorber with slowed carrier cooling properties and collection of carriers over a limited range of energies, such that cold carriers in the external contacts do not cool the hot carriers to be extracted (Conibeer et al., 2006). The contacts should be able to extract hot carriers from the solar cell at selective energy levels (Solanki and Beaucarne, 2007).

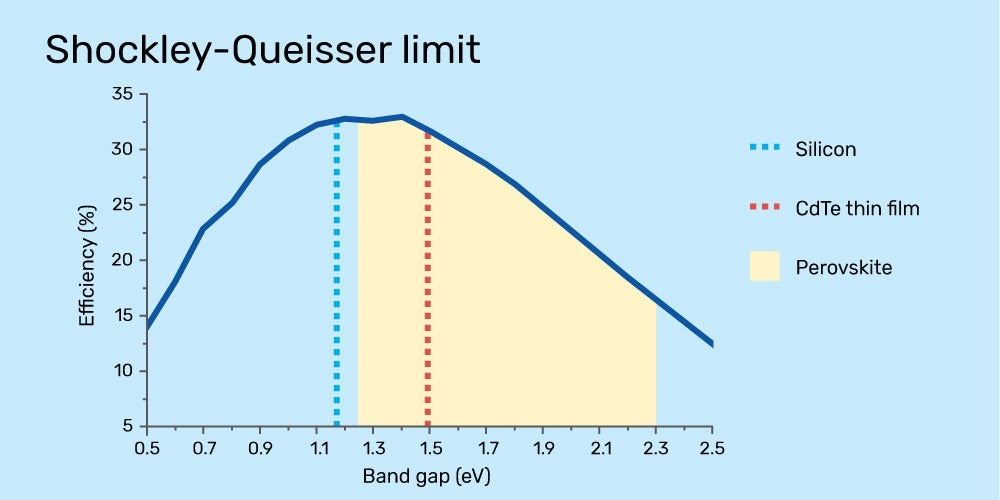
There is a gap between the Shockley-Queisser limit and the thermodynamic (Carnot) limit for evaluating solar cell efficiency heights. The Carnot efficiency limit for conversion of heat energy between the sun and the earth has been calculated at around 93.3% by Landsberg and Baruch (1989), considering radiative losses from the solar cell, and a black body limit of 86% considering the sun as a black body at 5760 K and a solar cell as another black body at, say, 300 K, taking into account entropy generation in the solar cell during the energy conversion, by Green (2003). So, why the large difference between the Shockley-Queisser and thermodynamic (Carnot) limits? This difference occurs because a single material is characterized by a single energy gap (the band-gap), whereas the solar spectrum contains photons with a wide range of energies, which means that devices that rely on a single transition between energy levels are not suited to the broad spectrum of sunlight. Strategies to overcome the Shockley-Queisser limit includesSpectrum splitting, or the splitting of the sun’s spectrum to be absorbed by many cells (e.g., multijunction solar cells, intermediate band solar cells, quantum well solar cells), reduction in thermalisation losses (e.g., hot carrier cells), or adapting the solar spectrum to one host material (e.g., up- and down-conversion of photon energy) (Solanki and Beaucarne, 2007).

The bulk photovoltaic effect (BPVE) in ferroelectric materials has also be considered as a way to break the physical limit of the Shockley-Queisser limit, as ferroelectric cells could outperform conventional semiconductor-based solar cells, because manipulating ferroelectric domains through AC poling yields a 35% increase in electric output. The BPVE in ferroelectric materials forms its own self-junction to harvest the solar energy and convert it into green electricity, whereas traditional semiconductor solar cells form p-n junctions. Balanov et al. (2025) discuss how Reorienting microscopic domains, tiny regions where electric polarizations align uniformly, within ferroelectric oxide perovskite crystals can significantly boost power output. Applying and removing an AC poling electric field would result in improved alignment, reducing the likelihood of charge carrier recombination, leading to a greater energy conversion efficiency. However, a material is needed that simultaneously has a narrow band gap (to maximise visible light absorption) and a large spontaneous polarization (Balanov et al., 2025; Shaikh, 2025). Solanki and Beaucarne (2007) define the impurity photovoltaic (IPV) effect as using two-step generation to leverage impurity states within the band gap to utilize sub-band-gap photons to generate electrical power by enabling transitions between impurity levels and the valence or conduction bands. An intermediate band (IB) solar cell is characterized by the existence of a narrow intermediate band within the main band-gap in order to increase the overall current generated while maintaining a high output voltage. In both the IPV effect and in IB cells, the same material is used throughout and the interconnection between cells occurs automatically.

A problem that arises with wide bandgap cells, however, is known as phase segregation, where different components separate over time, leading to a decline in device performance. Phase segregation is normally associated with ion migration behavior in the perovskites. Light-induced phase segregation is a problem which arises in perovskites with higher bromine concentrations, in which different bandgaps are formed within the same material, bromine-rich and iodine-rich regions. Light-induced phase segregation occurs when light falls on a wide bandgap material with a high bromine content, and the photoexcited charge carriers separate the halide ions resulting in the uneven distribution of halide ions (bromine-rich and iodine-rich regions) (Song et al., 2019). Swiss EPFL researchers have fixed this problem of phase segregation and stabilized wide bandgap cells by incorporating rubidium (Rb) using lattice strain and composition engineering, a controlled slight deformation in the atomic structure that helps keep rubidium in place in the perovskite lattice, boosting perovskite solar cells efficiency by minimizing non-radiative recombination. Another way to stabilize the lattice is to compensate for the size differences between the incorporated elements by introducing chloride ions, which ensures a more uniform distribution of ions, reducing defects and improving overall material stability (Zheng et al., 2025; Mirage News, 2025).

A Tauc plot is commonly used in the study of semiconductors to determine the optical bandgap of a material. The minimum energy required to excite an electron from the valence band to the conduction band, thus enabling light absorption, is known as the optical bandgap. To determine the bandgap on a Tauc plot, you must extrapolate the linear portion of the curve (usually after the absorption edge) to the x-axis (where the square root of the absorption coefficient is zero), and the corresponding photon energy at that point is the optical bandgap. ***Figure XXX*** shows the optical bandgaps of perovskite, silicon, and cadmium telluride.

Figure XXX.



Zientara, Ben (2025) Solar Reviews, Perovskite solar cells: why they’re the future of solar power,

<https://www.solarreviews.com/blog/are-perovskite-solar-cells-the-future-of-solar-power>

**Photon Absorption Management**

Perovskites were first used in dye-sensitized solar cells due to their superior absorption qualities. Materials with high absorption and high extinction (absorbs more light) require less material to collect incident light before it exits the back of the device. With an absorption coefficient over 10 times larger than that of silicon, perovskite solar cells can be approximately ten times thinner than a silicon solar cell to capture the same amount of light. The quantum efficiency is the ratio between the number of excited charge pairs produced for a specific number of incident photons, and must be the same for solar cell thickness scaling. Perovskite solar cells are extremely efficient at converting light into excited charge pairs, and have high quantum efficiencies due to their multiple methods of producing excited charge pairs.[[2]](#footnote-1) External quantum efficiency (EQE) measures the number of photons emitted or absorbed, while internal quantum efficiency (IQE) reflects the internal efficiency of charge generation and recombination. Perovskites can produce more electrons from the same thickness and number of incident photons than silicon, due to higher quantum efficiency and higher absorption, and thus perovskite cells can be thinner, lighter, and more flexible.

This band gap dictates which portion of the solar spectrum can be absorbed by a photovoltaic cell, as photons must match the bandgap, not be higher or lower (Goetzberger et al., 1998). A photon that has lower energy than the band gap energy will not be able to create enough excitation of the valence band electron to reach the conduction band, and thus the photon will not be absorbed. Conversely, when photons have higher energy than the band gap, they mostly generate heat by making a transition to the conduction band edge, and do not impact cell performance. Miah et al. (2024) considers three possible outcomes for when photons interact with a semiconducting material. One, depending on the difference in refractive index between the material and surroundings, they may be reflected from the surface. Two, depending on its extinction coefficient, they may be absorbed. Three, they may be transmitted through the material. Both reflection and transmission are considered losses in photovoltaic devices since photons are n ot absorbed and do not contribute to power generation. When a photon is absorbed, however, it can raise one electron from the valence band to the conduction band. The energy level of photons that will be absorbed is calculated in equation (1):

(1)

where represents the incident photon's energy and λ is the wavelength of the corresponding photon. Here, 1240 nm is the wavelength of a photon that contains 1 eV of energy. This incident photon will be absorbed if ≥ , where represents the band gap of the material. The highest absorption or emission occurs at the edge of the bandgap of semiconducting materials. There are three categories of incident photons based on their energy relative to the semiconductor band gap, and the absorption process.

(a) If the incident photon energy is smaller than the band gap energy , only minimal interactions with the semiconductor will occur (and such an interaction will not contribute to the photovoltaic process) and will pass through the material as if it is transparent.

(b) For = , the incident photons have just enough energy to produce an electron–hole pair and consequently, the valence band electron can just reach the conduction band.

(c) If the incident photon energy is larger than the band gap energy , strong photon absorption occurs and the electron now stays on the conduction band with some excess energy. However, in photovoltaic applications, additional photon energy with respect to the band gap is lost by the quick non-radiative transition of electrons to the conduction band edge. This non-radiative transition leads to heat generation.

As an example, it is well known that the AM 1.5G sunlight has a wide range of useable energy from ∼0.5 eV to 4.4 eV (wavelengths from 280 nm to 2500 nm) (Lei et al., 2022). The active perovskite materials used in PSCs typically have energy band gaps between 1.48 eV and 1.62 eV, where the optimum bandgap of the best-performing PSCs is almost pinpointed in the range from 1.53 eV to 1.56 eV (Jung et al., 2023; Hossain et al., 2021; Fujiwara et al., 2018A; Miao et al., 2021; Son et al., 2016; Yang et al., 2015; Saliba et al., 2016; Fujiwara et al., 2018B). It has been reported that the PSCs with a bandgap of ∼1.5 eV can utilize incident photons in the 300–800 nm region and photon absorption over 800 nm has been reported to be less (Eperon et al., 2014; Lei et al., 2022). This suggests that a significant portion of the solar energy over the near-infrared region cannot be utilized by the most recognized perovskites. The underutilization of high-energy photons is mainly related to hot carriers.

To address these issues, according to equation (1), the photon management concept can be employed (Zanatta, 2022). This approach involves modifying the band gap to align with the solar visible spectrum, which can tune the absorption profile of the solar-sensitive material, thereby optimizing its performance. In addition, the band-gap fine-tuning optimizes semiconductors for use as bottom or top cell absorbers in perovskite-based tandem cells for harnessing whole solar spectrum energy (Jiang et al., 2024B; Aydin et al., 2024; Priyanka and Muchahary, 2024). Various research groups have implemented diverse approaches including compositional engineering, dimensionality reduction, mixing of dimensions, and pressurized tactics to modulate the band gap in materials to align them with the solar spectrum (Noh et al., 2013; Eperon et al., 2014; Haq et al., 2021; Xing et al., 2018). These efforts have resulted in improved absorption, offering enhanced performance and heightened structural stability in solar energy conversion technologies (Xu et al., 2024).

Depending on the electronic band structure, there are two types of solar materials, namely, direct and indirect band-gap materials (Welte et al., 2008; Monllor-Satoca et al., 2007; Malyi and Acosta, 2020). In contrast to direct band gap materials, where electron transitions occur without momentum modification, indirect band gap materials necessitate the participation of a phonon to conserve momentum during electronic transitions, as shown in (Kangsabanik et al., 2022; Liang and Bowers, 2010). This additional requirement may meaningfully decrease the efficiency of photon absorption and the rate of electron–hole pair production, thereby controlling the performance of solar cells based on that material (Hutter et al., 2016). Moreover, the phonon-assisted transitions launch additional non-radiative recombination corridors for the generated electron–hole pairs (Haug, 1979; Pilkuhin, 1979). These non-radiative routes can significantly degrade the overall performance of solar cells based on indirect band gap materials (Green et al., 2014). Transforming indirect bandgaps into direct bandgaps and adjusting band structures to better match the solar spectrum improves the absorption of sunlight and facilitates more efficient charge carrier generation.

Spectral conversion and plasmonic effects are two ways to increase photon absorption. If the photons in the solar spectrum were all the same energy as bandgap, such as 1.12 for silicon, then the energy efficiency of the cell would greatly increase. Spectral conversion is the process of using material layers to change high-energy photons (~3 eV) and low-energy photons (~0.3 eV) in the solar spectrum for either up-conversion, converting two or more low-energy photons into a higher-energy photon (placed at the top of the cell from where light is entering the cell to avoid thermalization losses), or down-conversion, converting one high-energy photon into two or more lower-energy photons (placed at the bottom or rear side of the cell with a reflector). Surface plasmon is defined as the collective oscillation of the electrons in the conduction band confined to the surface. The surface plasmon can be excited by incident photons in a small metallic structure coated on a dielectric surface when the size of the metallic particles at the surface is much smaller than the photon wavelength. Surface plasmon can improve the absorption of light in thin film cells due to local electromagnetic field enhancement (Schaadt et al., 2005; Stenzel et al., 1995), and can also be used to improve the efficiency of up-conversion and down-conversion materials.

**Band-gap Tuning, Compositional Engineering**

-approaches for achieving high performance and stability of PSCs by band gap alteration

1. Substituting A-site Cations
2. Substituting B-site Cations
3. Substituting X-site Anions
4. Pressure
5. Reducing Dimension

In a perovskite structure with the formula , "A" typically represents a larger, monovalent cation like Cs+ (cesium), MA+ (methylammonium), or FA+ (formamidinium), "B" is a smaller, often divalent metal cation like Pb2+ (lead) or Sn2+ (tin), and "X" is a halide anion such as Cl- (chloride), Br- (bromide), or I- (iodide). Methylammonium cations (MA+) are positively charged organic molecules acting as the "A" cation in the perovskite crystal structure, where they play a crucial role in influencing the material's optical and electrical properties, contributing to efficient light absorption and charge carrier transport within the solar cell; however, their use can be limited due to potential stability concerns related to their relatively small size and polar nature. When combined with inorganic halide anions (like iodine) and a metal cation (like lead), methylammonium forms the perovskite crystal structure, crucial for light absorption in the solar cell. To address stability issues, researchers often blend methylammonium with other cations like formamidinium (FA+) to create "triple cation" perovskites, offering improved stability while maintaining high efficiency.

The band gap is the energy difference between the valence band maximum and the conduction band minimum of a material. Because of its direct influence on optoelectronic characteristics, band-gap adjustment in perovskite materials is crucial. It specifies the range of light wavelengths that a substance may absorb and convert into an electrical signal. The ability to modify the band-gap from low to high range has made perovskites appealing for a diversity of applications including photovoltaics, lasing, light-emitting devices, photodetectors, high energy, and particle detection (Miah et al., 2024). Metal halide perovskites are an encouraging family of materials for highly efficient PSCs for their tunable band-gap aligning with solar energy. In this section, compositional engineering, pressure-induced band gap modulation, and dimensional reduction and mixing approaches have been discussed.

Compositional engineering involves replacing elements in different sites in , where B and X-site modifications have more pronounced effects on the electronic band gap structure as compared to A-site replacement. While A-site replacements mainly influence the spatial arrangement of octahedral structures, B and X-site replacements directly impact the conduction and valence bands of the perovskite materials, respectively. Consequently, strategies focusing on B and X-site modifications are more effective for attaining desired band gap adjustments.

However, although pressure-induced bandgap tailoring effectively modifies the bandgap of perovskite materials, there are issues connected with maintaining a consistent pressure during the device's application to attain optimal performance levels. This drawback raises concerns about the practical viability and long-term stability of devices relying solely on pressure-induced modulation.

perovskite-based tandem solar cells (PBTSCs)

***Compositional Engineering***

One of the most appealing aspects of perovskites for photovoltaics is the capability to adjust their energy band gap by simple compositional exchange. The perovskite semiconducting materials utilized in high-performing PSCs typically have energy band gaps between 1.48 eV and 1.62 eV (Eperon et al., 2014; Son et al., 2016; Saliba et al., 2016; Yang et al., 2015). The semiconducting materials with lower band gaps are essential for capturing more of the visible solar spectrum. Utilizing different perovskite materials with varying band gaps enables the formation of PBTSCs, permitting the absorption of a wider spectrum of light. This approach has the potential to exceed the Shockley–Queisser PCE limit observed in single-junction PSCs (Shockley and Queisser, 1961). As an extensively used and high PCE-possessing material, the energy band-gap of methylammonium lead iodide () may be adjusted from 1.6 eV to 2.3 eV by replacing iodine with bromine at different ratios (Noh et al., 2013). A similar technique may adjust the band gap of formamidinium lead tri-halide () from 1.48 eV to 2.23 eV.21 The compositional band-gap fine-tuning optimizes metal halide perovskites for usage as bottom or top cell absorbers in tandem or single junction solar cells. A-site substitution has a relatively less direct impact on the edge of the band structure, i.e., Eg in comparison with B and X-site substitutions in the phases (Lehner et al., 2015). However, A-site cations can influence the lattice constant, which might indirectly influence the band structure. These A-site cations can also affect the dielectric characteristics, hydrogen bonding interactions (with halide anions), and/or alter the octahedral framework. We have outlined the following three factors involved with the compositional changes, which may facilitate the readers' understanding of the band gap engineering of the perovskite materials.

(i) The first aspect is related to electronegativity, where is increased when the electronegativity difference between the B-site metal and the X-site halide increases, but the A-site atoms have an indirect effect on . (Kim et al., 2015A; Kim et al., 2016A).

(ii) The second factor linked to the is the B–X–B angle. Particularly, increases with the B–X–B angle decreases (Filip et al., 2014; Amat et al., 2014).

(iii) The third factor is the distance between X and B atoms, where is reduced as the distance between the X and B atoms decreases (Kim et al., 2015A; Grote and Berger, 2015; Kong et al., 2016).

It is essential to emphasize that when replacing atoms at various sites within the structure, careful attention must be given to maintaining the Goldschmidt tolerance factor and octahedral factor in order to achieve and preserve the 3D crystal structure. It is generally well-known that the characteristics of a semiconducting material are substantially governed by its crystal structure; hence, geometric distortion considerably contributes to the modifications in the features of perovskite semiconducting materials.

In perovskite solar cells, a Type-I band alignment, also known as a step-down band alignment, is used to efficiently block minority carriers and promote charge separation. This alignment ensures that the minority carriers (e.g., electrons in an n-type material) are blocked at the interface between different layers, preventing them from recombining and increasing the overall efficiency of the solar cell.

Here's a more detailed explanation:

Minority Carriers:

In a solar cell, minority carriers are the charge carriers that are not in the majority (e.g., electrons in an n-type material or holes in a p-type material).

Type-I Band Alignment:

In a Type-I band alignment, the conduction band of one material is lower in energy than the conduction band of another material, and similarly, the valence band of one material is lower in energy than the valence band of another material. This creates a "step-down" in the energy levels at the interface.

Blocking Minority Carriers:

Because of this "step-down," when a minority carrier reaches the interface between two materials with a Type-I band alignment, it is blocked from moving into the other material. This is because it would require too much energy to overcome the potential barrier.

Charge Separation and Efficiency:

By blocking minority carriers, the Type-I band alignment helps to promote the separation of charge carriers (e.g., electrons and holes) in the perovskite solar cell, which are then extracted as current. This leads to higher efficiency in converting light into electricity.

In summary, Type-I band alignment plays a crucial role in perovskite solar cells by efficiently blocking minority carriers, promoting charge separation, and ultimately enhancing the overall efficiency of the device.

Pazos-Outón, L.M., Xiao, T.P., and Yablonovitch, E. (2018) Fundamental Efficiency Limit of Lead Iodide Perovskite Solar Cells, J. Phys. Chem. Lett., 9(7), 1703–1711, DOI:10.1021/ACS.JPCLETT.7B03054/ASSET/IMAGES/LARGE/JZ-2017-030546\_0008.JPEG.

It has been known that under 1-sun illumination the efficiency limit of crystalline silicon is ∼29%, despite the Shockley–Queisser (SQ) limit for its bandgap being ∼33%: the discrepancy is due to strong Auger recombination. In this article, we show that methyl ammonium lead iodide (MAPbI3) likewise has a larger than expected Auger coefficient. Auger nonradiative recombination decreases the theoretical external luminescence efficiency to ∼95% at open-circuit conditions. The Auger penalty is much reduced at the operating point where the carrier density is less, producing an oddly high fill factor of ∼90.4%. This compensates the Auger penalty and leads to a power conversion efficiency of 30.5%, close to ideal for the MAPbI3 bandgap

For any technology to approach the theoretical limit laid out by Shockley and Queisser, (Shockley and Queisser, 1961) the device must be designed not only for the efficient collection of photogenerated carriers, but also for the efficient extraction of internal luminescence (Miller et al., 2012) The first barrier of entry for a high performance photovoltaic technology is efficient carrier extraction. Once this is achieved, light management becomes the limiting factor for device efficiency. Good light management manifests itself in an improved short-circuit current by enhancing the material’s absorptivity to incident sunlight. A yet more important consequence of good light management in a solar cell is an increase in its open-circuit voltage (and hence the operating voltage). The degree to which a solar cell’s voltage approaches ideal is directly related to its ability to extract its own internal luminescence, as derived in 1967 by Ross: (Ross, 1967)

where is the expected open-circuit voltage, is the radiative (ideal) limit of the open-circuit voltage, and ηext is the external photoluminescence quantum efficiency (PLQE). The radiative limit assumes that all recombination processes are radiative and that every luminescent photon escapes the solar cell. We distinguish it from the Shockley-Queisser limit, which additionally assumes that the material is a hypothetical step-function absorber at the band edge.

It is important to note that, unlike the SQ limit, the ideal radiative voltage, , is not a constant of the material, as it also varies with the optical design. When accounting for the properties of real materials, which can have weak but nonzero absorption below the band edge, the optical design of the device can change the effective bandgap. (Miller et al., 2012; ,Ren et al., 2017) As an example, we can consider two distinct effects that texturing a solar cell will have on its performance: On one hand, it increases the absorptivity at long wavelengths, which produces a red-shift of the effective bandgap. This will produce an enhancement of the short-circuit current and a reduction of the voltage, . In effect, the device will operate as a solar cell with a slightly smaller bandgap. On the other hand, texturing favors light extraction, increasing the external luminescence efficiency. This gain in external luminescence efficiency increases the open-circuit voltage, , bringing it closer to the ideal voltage, . Therefore, any enhancement in the external luminescence efficiency is beneficial for device performance.

The reasoning behind eq 1 is the following: by the law of mass action for semiconductors, the internal quasi-Fermi level separation in a solar cell is proportional to the logarithm of the carrier density product, np. The steady-state carrier density is determined by the balance between carrier injection and carrier decay. Under open-circuit conditions, where no charge carriers can be extracted by the electrodes, carriers are removed from the semiconductor through (1) radiative recombination, and subsequent escape out of the device as photons, (2) internal nonradiative recombination, or (3) parasitic absorption, after being converted to internal photons. The first is a necessary phenomenon since, as dictated by detailed balance, (5) the absorptivity and the emissivity are directly linked. Because light must enter the solar cell from the front surface, the extraction of internally generated photons through the same surface cannot be blocked. This process determines the minimum possible rate of carrier loss. Therefore, the only way to maximize carrier density is by minimizing nonradiative recombination and internal photon losses. The result of minimizing these losses is the maximization of the external luminescence efficiency, which translates into an enhanced open-circuit voltage as given by eq 1.

In order to determine the fundamental efficiency limit of lead halide perovskites, we need the intrinsic recombination rates, similar to prior fundamental efficiency analysis on GaAs (Miller et al., 2012) and crystalline silicon (Tiedje et al., 1984) The only intrinsic recombination processes are radiative recombination and Auger recombination. We will call the efficiency in the presence of these two processes the “Auger limit”, in contrast to the “perfect radiator” radiative limit, which includes only radiative recombination. Shockley–Read–Hall (SRH) recombination is a nonfundamental decay channel mediated by defects, and is excluded from our intrinsic efficiency limit calculation. This is justified since the usefulness of the lead halide perovskites can be attributed to the surprisingly small SRH recombination.

Disregarding all forms of nonradiative decay, the radiative limit can be derived from the detailed-balance approach used by Shockley and Queisser, (Shockley and Queisser, 1961)) which invokes the equality of absorptivity and emissivity at all energies E: a(E) = ε(E). Rather than a step function absorber, as assumed in the original SQ work, we use the real absorptivity spectrum of perovskite materials. When constrained by the actual absorption spectrum, the radiative limit (Sha et al., 2015) provides a reference versus the real performance limit, which includes both radiative recombination and Auger nonradiative recombination.

Sha, W. E. I.; Ren, X.; Chen, L.; Choy, W. C. H. The Efficiency Limit of CH3NH3PbI3 Perovskite Solar Cells. Appl. Phys. Lett. 2015, 106, 221104, DOI: 10.1063/1.4922150

Tiedje, T.; Yablonovitch, E.; Cody, G. D.; Brooks, B. G. Limiting Efficiency of Silicon Solar Cells. IEEE Trans. Electron Devices 1984, 31, 711– 716, DOI: 10.1109/T-ED.1984.21594

Ren, X.; Wang, Z.; Sha, W. E. I.; Choy, W. C. H. Exploring the Way to Approach the Efficiency Limit of Perovskite Solar Cells by Drift-Diffusion Model. ACS Photonics 2017, 4, 934– 942, DOI: 10.1021/acsphotonics.6b01043

Miller, O. D.; Yablonovitch, E.; Kurtz, S. R. Strong Internal and External Luminescence as Solar Cells Approach the Shockley–Queisser Limit. IEEE J. Photovoltaics 2012, 2, 303– 311, DOI: 10.1109/JPHOTOV.2012.2198434

Ross, R. T. Some Thermodynamics of Photochemical Systems. J. Chem. Phys. 1967, 46, 4590– 4593, DOI: 10.1063/1.1840606

**Recombination Mechanisms**

In solar cells, recombination mechanisms refer to the ways electron-hole pairs generated by light absorption can return to a state of thermal equilibrium by recombining, essentially "rejoining" to release energy. This process is the opposite of charge carrier generation, where photons excite electrons, separating them from their respective holes. Recombination is a natural process and an intrinsic property of any semiconductor material, and occurs when the electron meets a hole and completes a broken bond. When a solar cell absorbs light, it generates electron-hole pairs. These pairs represent the excess charge carriers created by the light. Without recombination, these excess carriers would accumulate and create a non-equilibrium state. Recombination acts to return the material to its thermal equilibrium state. During recombination, electrons and holes recombine, and the excess energy is released. This energy can be released in various forms, including as heat or light (in LEDs). In essence, recombination mechanisms describe how the energy from absorbed light is lost in a solar cell, either as heat or by other means, and how this affects the cell's ability to generate electricity.

There are different recombination mechanisms: the band to band radiative recombination, the band impurity band Shockley–Read–Hall nonradiative recombination, and Auger recombination. Non-radiative recombination occurs when an electron and a hole recombine, but instead of emitting a photon (as in radiative recombination), the energy is released as heat or transferred to the lattice structure. Non-radiative recombination reduces the efficiency of a solar cell because it reduces the number of free carriers (electrons and holes) available to generate electricity. Radiative recombination is a process where an electron and a hole recombine, releasing energy in the form of a photon. Auger recombination involves the interaction of three carriers (two electrons and one hole) to create energy transfer without photon emission. Shockley-Read-Hall (SRH) Recombination involves carrier recombination through defects or traps (intermediate states) within the semiconductor material. Grain boundaries in perovskite films can act as defect states, creating traps for charge carriers. Intrinsic defects like antisites, interstitials, and vacancies can also form defect states. Surface defects at the edges of perovskite films can also lead to non-radiative recombination

Fundamental performance limits were analyzed using a realistic detailed balance model with measured optical properties and several recombination mechanisms, including defects. The scientists used a balance model incorporating measured optical properties as well as radiative, Auger, and Shockley-Read-Hall (SRH) recombination, as well as various indoor light sources, including compact fluorescent lamp (CFL), light-emitting diode (LED), halogen, and low-intensity AM 1.5 G lighting (Nitta et al., 2025; Bellini, 2025W).

However, the main nonradiative recombination mechanism is the defect-assisted Shockley–Read–Hall (SRH) recombination in PSCs, in which the defect density at the interfaces is approximately two orders of magnitude higher than that of the bulk perovskite films (Ni et al., 2020; Chen and Zhou, 2020) Additionally, the recombination at the surfaces/interfaces is faster than that inside bulk films, and thus the total carrier lifetime in polycrystalline perovskite films is often limited due to the surface recombination (Yang et al., 2017). Therefore, surface passivation for the reduction of nonradiative recombination is required to further improve the devices’ performance (Jeong et al., 2021).

**Contact Passivation**

The interaction between the passivation molecules and the different perovskite crystal facets is critical to achieving a uniform passivation layer on the whole perovskite surface. A facet-dependent passivation principle. Is useful for determining the dependence of crystal facets on passivating materials. Contact passivation in perovskite solar cells involves treating the interface between the perovskite layer and the contacts (electron and hole transport layers) to reduce defects and improve charge extraction. This is achieved by using materials that either chemically interact with the perovskite to fill trap states or physically block recombination. Passivation enhances efficiency and stability by mitigating defects and improving carrier transport. Passivation can be used for defect mitigation in perovskite solar cells, which often suffer from defects in the perovskite layer, such as grain boundaries and surface states, which can lead to non-radiative recombination and reduced performance. Passivation layers can improve the interface between the perovskite and the transport layers, facilitating better charge carrier extraction (electrons or holes). In 2D/3D perovskite heterojunctions, integrating 2D perovskites on the surface of 3D perovskite can act as a passivation layer, improving charge transport and suppressing recombination. Surface passivation can be achieved with organic molecules, as small organic molecules or polymers can be used to fill surface defects and reduce non-radiative recombination. Inorganic compounds like PbS can be used to reduce interfacial defects and improve crystallization. Organic HTMs with passivation groups can directly passivate the perovskite surface. Passivation leads to higher power conversion efficiency (PCE) and better open-circuit voltage (Voc). Interface passivation can reduce hysteresis in the current-voltage (J-V) curves. Passivation can lead to improved device stability under ambient conditions and thermal aging.

Jeong, S., Seo, S., Yang, H., and Park, H. (2021) Cyclohexylammonium-Based 2D/3D Perovskite Heterojunction with Funnel-Like Energy Band Alignment for Efficient Solar Cells (23.91%). Adv. Energy Mater., 11, 2102236.

Ni, Z., Bao, C., Liu, Y., (2020) Resolving spatial and energetic distributions of trap states in metal halide perovskite solar cells, Science, 367, 1352;

Chen, Y.H. and Zhou, H.P. (2020) Defects chemistry in high-efficiency and stable perovskite solar cells, J. Appl. Phys., 128, 060903.

Yang, Y., Yang, M.J., Moore, D.T., et al. (2017) Top and bottom surfaces limit carrier lifetime in lead iodide perovskite films, Nat. Energy, 2, 16207.

**Minimizing Bulk and Surface Defects in Perovskite Cells**

The positive (holes) and negative (electrons) charges must be separated and drawn into their respective transport layers, and bulk and surface defects within the perovskite crystal act as recombination centers for the charge carriers and reduce the number of excited charges collected in the circuit. This means that quantum efficiency does not directly translate into power conversion efficiency.[[3]](#footnote-2)

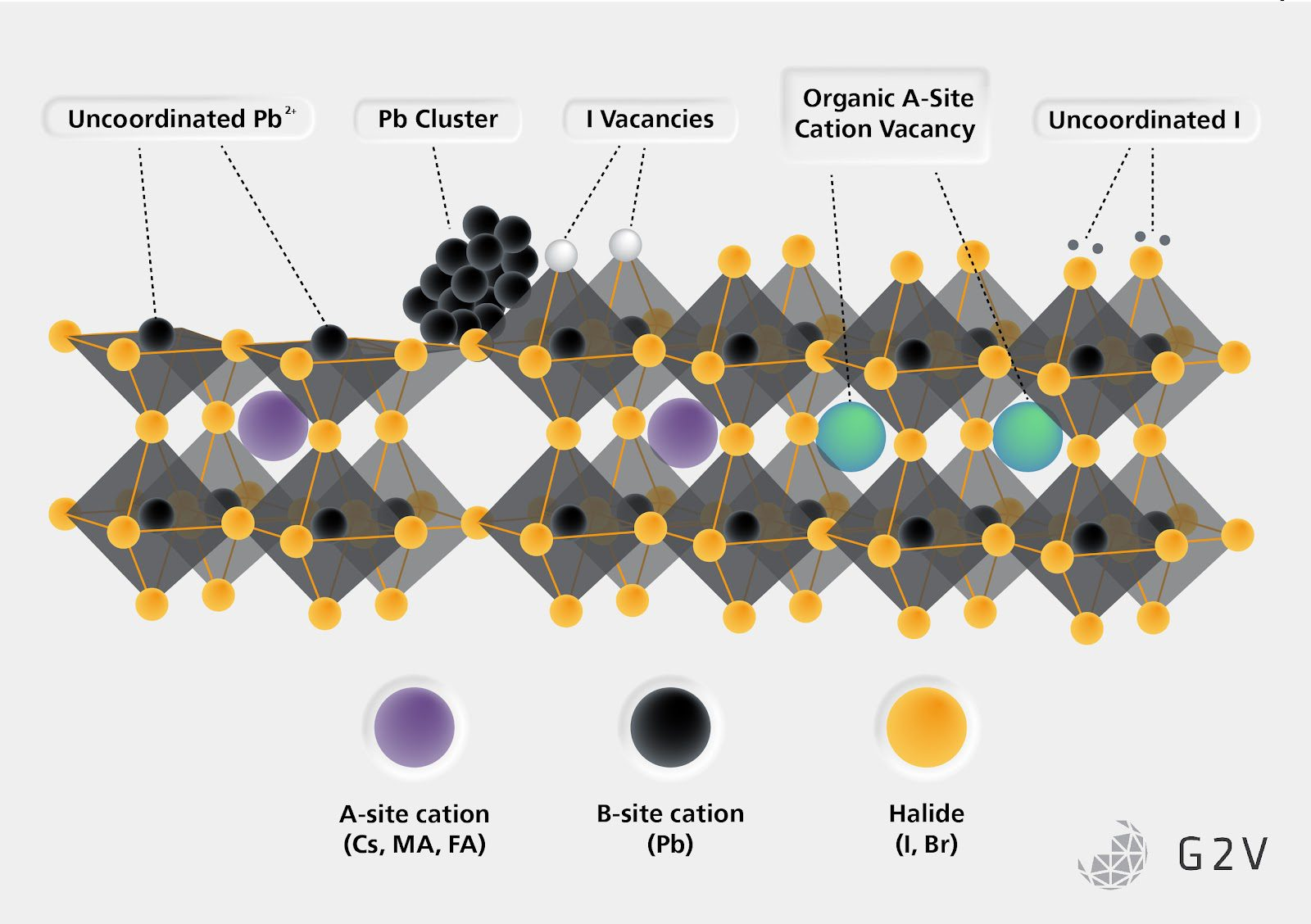
These bulk and surface defects are also known as trap states, are found in the absorber layer, hole transport layer (HTL), and electron transport layer (ETL), and which form on the surface of the perovskite film and at grain boundaries during the fabrication of the perovskite film, and restrict the performance and stability of PSCs by allowing the entry of oxygen and moisture into the perovskite film. Passivating the perovskite film, which is aimed at stabilizing the material’s surface and interfaces, includes additive engineering, interface engineering, and antisolvent engineering, and results in the formation of a hydrophobic film with few defects, good crystallinity, and large grain size (Boro et al., 2022; deQuilettes et al., 2024; Lewis, 2024).

Defects represent a deviation from a perfect crystal in the desired stoichiometric ratio or geometric pattern. Defects require either more energy to get over (blocking low voltage charges), or more time spent to get around (increasing the required lifespan of the mobile charge to reach a current collector, so fewer charges make it before recombining, lowering the output current). Defects impact how current flows through the material by impacting the local stress on the crystal and the local electric fields.

Bulk defects are errors within a single crystal such as missing atoms, extra atoms, impurities, atoms in the wrong spot, and so on, and are the outcome of being unable to create a crystal perfectly atom by atom. However, some bulk defects allow for better ion transport mobility, as with a perfect lattice every position for every mobile ion is perfectly filled within a perovskite crystal, and the amount of energy required to move ions is increased since any incoming ion has to first knock out the atom already occupying the space. Perovskites are generally insensitive to bulk defects because there are multiple charge separation/transport methods through the bulk materials, meaning you have multiple different interactions with any defects, and there is high mobility of the X position atoms within the lattice, which allows charges to ignore most of their electronic effects during operation, because defects are unlikely to stay in one position for very long, meaning defects are spread over a larger volume and thus have a lower severity of interaction over that volume.

Surface defects are defects arising from a mismatch in the atomic lattices either between different materials or within the same material type, such as a crystal lattice mismatch at the interface between a CTL and the perovskite or a grain boundary between two crystal grains within a perovskite. The surface in surface defects refers to the contact points between two or more lattice-mismatched crystals or materials, not external surfaces. A surface defect can act as a trap for charges by changing the local internal electric field by diverting charges from being properly collected and used in the circuit of the solar cell, also known as non-radiative recombination, or surface recombination. In non-radiative recombination, the charges, either holes or electrons, within the defect attract and combine with their opposite charges in the crystal preventing the charge from making it to the electrode.

Figure XXX.



Some examples of bulk defect types in perovskites. Not shown are interstitial defects where extra atoms are wedged in between properly placed atoms.

Lu, H., Krishna, A., Zakeeruddin, S., Grätzel, M., and Hagfeldt, A. (2020). Compositional and Interface Engineering of Organic-Inorganic Lead Halide Perovskite Solar Cells. iScience. 101359,

<https://www.researchgate.net/publication/342861512_Compositional_and_Interface_Engineering_of_Organic-Inorganic_Lead_Halide_Perovskite_Solar_Cells>

**Effects of Different Cations and Anions on Perovskite Properties**

Substituting different cations at the A and B sites of the perovskite structure (AX2B) can significantly impact the material's crystal structure, band gap, stability, charge carrier mobility, and overall optoelectronic properties. Changing the size and charge of the A-site cation (e.g., substituting smaller cations like Cs+ for larger ones like MA+) can influence the lattice distortion, impacting the stability and optical properties of the perovskite. Modifying the B-site cation (e.g., Pb2+ with Sn2+) can significantly alter the band gap, affecting the absorption spectrum and charge carrier mobility. Substituting different halide anions (I-, Br-, Cl-) at the X-site can significantly adjust the band gap due to their varying electronegativity, allowing for fine-tuning of the perovskite's optical properties. Incorporating larger cations like Cs+ can enhance the structural stability of the perovskite by reducing lattice distortions. Using a mixture of cations with different sizes (e.g., MA+ and FA+) can sometimes lead to better stability by creating a more evenly distributed strain within the lattice. Halide substitution can be used to tune the bandgap, such as replacing I- with smaller Br- or Cl- anions, which can lead to a wider bandgap, shifting the absorption spectrum towards shorter wavelengths. The choice of A-site cation can affect the charge carrier mobility due to the interaction with the lattice vibrations. Intentionally introducing small amounts of dopant cations can help passivate defects, improving the perovskite's electrical properties. The properties of hybrid perovskites, such as MAPbI3, depend on various types of interactions and structural disorders. The interaction between the organic cation and the halide anion (for example, the NH3+ group of the MA cation and the halide atoms in MAPbX3) in perovskite is determined by the hydrogen bonding between them (Boro et al., 2022).

**Material, Strain, and Compositional Engineering**

**Material Engineering**

Material engineering helps to enhance the performance and stability of perovskite solar cells (PSCs) by optimizing the chemical composition, morphology, and interfaces of the perovskite absorber layer and other cell components. Material engineering for perovskite cells can be broken down into three categories: 1) perovskite absorber layer engineering 2) interface engineering 3) device architecture and fabrication. Perovskite absorber layer engineering can include either compositional tuning or morphology control. Within compositional tuning/engineering, there is the ability to engineer A-site cations, B-site cations, and X-site cations. You can also create mixed perovskites, such as FA and MA, and can conduct surfactant engineering, where cationic surfactants can be used to regulate perovskite crystallization, reducing charge trap density, and improving carrier lifetime. For morphology control, the perovskite film's grain size and morphology can be optimized, film thickness can be controlled, and the surface can be passivated, which is where the surface is treated with specific materials (Prakash et al., 2018; Bakr et al., 2017).

Interface engineering can include modifying either the electron transport layer (TiO2, MXenes) or the hole transport layer (PEDOT:PSS, spiro-OMeTAD). Passivating the interface with suitable materials can reduce recombination and improve device performance. Strain engineering can also be used, as modulating the strain nature and its gradient over the perovskite film can improve hole carrier transport and extraction across the interface of perovskite absorber/HTM.

Device architecture and fabrication can refer to device configuration, fabrication techniques, or scaling up manufacturing. Exploring different device architectures (e.g., planar, inverted) can optimize charge transport and stability. Developing low-cost and scalable fabrication methods (e.g., ink-jet printing, spin coating) is critical for commercialization.

**Strain Engineering**

Strain is the structural deformation of a material’s crystal lattice when the material is applied with a stress, external or internal. Internal forces leading to strain include defects, bulk or surface, including interstitials and vacancies. There are four types of strain investigated in perovskites: 1) compressive strain, squeezing together 2) tensile strain, pulling apart 2) microstrain, defects 3) atomic displacement vectors. Compressive strain occurs when the material contracts by external pressures, and enhances stability and improves charge transport, thereby increasing the activation energy or resistance for ion migration, which can reduce defect formation and improve thermal and light stability of perovskite solar cells. Tensile strain is when the material is stretched by external forces, and can weaken atomic bonds and reduce stability, by reducing the energy required for and increasing ion migration and weakening bonds, leading to degradation of the perovskite. Microstrains need to be reduced, and are a result of internal forces, and leads to an irregular twist inside of the crystal structure (Tao, 2022).

Strain engineering modulation strategies include: compositional tuning, film formation control, additive engineering, and interface engineering. Compositional tuning involves adjusting or tuning the chemical composition of the precursor perovskite material, such as introducing other ions like Cs and Cl, to control lattice parameters and reduce microstrain. The added ions could be either in A position or halide position (X). For film formation control, thin-film deposition techniques such as annealing or solvent engineering can be optimized to manage crystallization and reduce microstrain. Introducing additives can modify the perovskite's crystal structure and relieve or induce specific strain states. Additives can include dopants, solvents, or facets. Interfaces between perovskite layers and other materials need to be optimized to minimize lattice mismatches induced by the difference of coefficient of thermal expansion (CTE) between layers and microstrain.

**Compositional Engineering**

Compositional engineering in perovskite solar cells involves modifying the chemical composition of the perovskite material to optimize its properties, such as bandgap, stability, and charge transport, ultimately improving the efficiency and performance of the solar cell. Compositional engineering addresses the challenges of stability under environmental conditions and lead toxicity by fine-tuning the perovskite material's composition to achieve desired properties. Tuning the bandgap and charge transport properties can lead to higher power conversion efficiencies. Compositional engineering allows for the development of perovskite materials with tailored properties for specific applications, such as flexible solar cells or tandem solar cells. Compositional engineering strategies include: modifying the A-site cation, modifying the B-site cation, modifying the X-site cation, and tuning the perovskite composition. In FA1-xMAxPb(I1-yBry)3, FA and MA are mixed cations and I and Br are mixed anions, is a common example of compositional engineering used to improve stability and efficiency. Challenges encountered in compositional modification of perovskite devices include the significantly shortened carrier lifetime (∼50 ps), and thus, considerable loss of photovoltage upon the replacement of Pb by Sn, or the largely widened band gap, and hence, weaker light absorbance when I is substituted with Br or Cl, or interior stability due to the substantial substitution of I with Br (Parrott et al., 2016; Shi et al., 2015; Brenner et al., 2016; Liu et al., 2019A).

**Material Engineering**

Bakr, Z.H., Wali, Q., Fakharuddin, A., et al. (2017) Advances in hole transport materials engineering for stable and efficient perovskite solar cells, Nano Energy, Volume 34, Pages 271-305, <https://doi.org/10.1016/j.nanoen.2017.02.025>

**1. Perovskite Absorber Layer Engineering:**

***A) Compositional Tuning:***

1. A-site cation engineering: Modifying the A-site cations (e.g., methylammonium (MA), formamidinium (FA), caesium (Cs)) in the ABX3 perovskite structure can tailor the bandgap and optoelectronic properties.
2. B-site cation engineering: Exploring lead-free perovskites by replacing lead with tin (Sn), germanium (Ge), or other metals can improve stability and reduce toxicity.
3. X-site anion engineering: Using different halide anions (e.g., iodide (I), bromide (Br), chloride (Cl)) or pseudo-halide anions (e.g., formate (HCOO)) can influence defect passivation and charge transport.
4. Mixed perovskites: Combining different perovskite compositions (e.g., FA and MA) can enhance stability and performance.
5. Surfactant engineering: Using cationic surfactants can regulate perovskite crystallization, reduce charge trap density, and improve carrier lifetime.

***B) Morphology Control:***

1. Grain size and morphology: Optimizing the perovskite film's grain size and morphology can improve charge transport and reduce recombination.
2. Film thickness: Controlling the thickness of the perovskite layer is crucial for efficient light absorption and charge extraction.
3. Surface passivation: Surface passivation refers to the process of treating the perovskite surface with specific materials to reduce surface defects and enhance device stability.

**2. Interface Engineering:**

1. ***Electron Transport Layer (ETL)/Perovskite Interface:***
2. Work function tuning: Engineering the interface between the ETL (e.g., TiO2, MXenes) and perovskite can optimize electron injection and extraction.
3. Interface passivation: Passivating the interface with suitable materials can reduce recombination and improve device performance.
4. ***Hole Transport Layer (HTL)/Perovskite Interface:***
5. Interface engineering: Optimizing the interface between the HTL (e.g., PEDOT:PSS, spiro-OMeTAD) and perovskite can enhance hole extraction and transport.
6. Strain engineering: Modulating the strain nature and its gradient over the perovskite film can improve hole carrier transport and extraction across the interface of perovskite absorber/HTM.

**3. Device Architecture and Fabrication:**

1. ***Device configuration:***

Exploring different device architectures (e.g., planar, inverted) can optimize charge transport and stability.

1. ***Fabrication techniques:***

Developing low-cost and scalable fabrication methods (e.g., ink-jet printing, spin coating) is crucial for commercialization.

1. ***Scale-up and large-area device fabrication:***

Developing methods for fabricating large-area devices with high efficiency is essential for practical applications.

**Strain Engineering**

Internal forces leading to microstrains include defects within the material, lattice mismatches between the perovskite film and substrate, compositional changes or variations in the composition of the perovskite film, film thickness, phase transitions, and grain boundaries. External factors include environmental factors and thermal stress, the thermal expansion coefficient differences between the perovskite film and substrate during fabrication. During film formation, if the substrate has a low coefficient of thermal expansion (CTE), tensile strain would form because the substrate restricts the contraction of perovskite. Conversely, if the CTE of the substrate is higher than the film, compressive strain would form. Heteroepitaxy, where a crystalline film is grown on a substrate made of a different material, can lead to a mismatch inducing strain. The interplanar spacing (d) of the substrate determines whether the strain is tensile or compressive. However, if the difference of (d) is too large, it will lead to an uniformed, distorted interface. As for environmental factors, when perovskite devices are exposed to light during operation, some microstrain might occur. Grain boundaries are another creator of microstrain, which results from the different orientation of the same crystal structure, or interfacial strain field between grains (Tao, 2022).

Strain mechanism engineering can be used to increase the stability of perovskite crystals and to improve perovskite’s performance. Strain is both applied when fabricating, and is also influenced by environmental factors. To improve perovskite devices’ performance and stability, we must understand how strains form and which factors affect strains, then use characterization analysis to determine methods to either utilize compressive/tensile strain or reduce microstrain. Strain can significantly influence the optoelectronic properties of perovskites, affecting: bandgap, charge carrier mobility, defect formation, ion migration, and overall stability. Strain engineering can produce enhanced stability, improved efficiency, and controlled properties. Controlling strain can reduce defect formation and ion migration, leading to improved long-term stability of PSCs. Optimizing strain can enhance charge carrier transport and reduce recombination losses, resulting in higher power conversion efficiencies. Strain engineering can control properties, such as fine tuning the band gap of the perovskite material. It has been noted that when the perovskite material is applied with tensile strain, its bandgap increases, and when applied with compressive strain, the bandgap decreases. Carrier mobility decreases with more dislocations by the higher magnitude of strain applied, though the A ion’s stacking pattern could be tuned, in order to reduce the interaction between phonons and electrons. Compressive strain could be applied in order to increase the ion migration activation energy, however, according to Poisson’s effect, when the film is applied compressive strain horizontally, it would have tensile strain in perpendicular direction, which would also lead to cracks and unsmooth texture (Tao, 2022).

**Examples**

1. Formamidinium-based perovskites: In-plane compressive strain can stabilize formamidinium-based perovskites in PSCs.
2. Quantum Dot-in-matrix perovskites: Quantum dot embedding can induce compressive strain, improving the stability of perovskite solar cells.
3. DBDA additive: The addition of 2,2-diamino-[1,1-biphenyl]-4,4-dicarboxylic acid (DBDA) can help to convert tensile stress into compressive strain.

Accurate characterization analysis is needed for effective strain engineering, and includes techniques like X-ray diffraction (XRD), Raman spectroscopy, electron backscatter diffraction (EBSD), transmission electron microscopy (TEM), atomic force microscopy (AFM), scanning electron microscopy (SEM), and density functional theory (DFT). XRD can be used to analyze both in-plane and out-of-plane strain, and determines the crystal structure and lattice parameters of the perovskite material, assessing strain by comparing the positions of diffraction peaks in a strained sample to a reference sample. Under XRD, compressive strain shifts diffraction peaks to higher angles, while tensile strain shifts them to lower angles. Grazing Incidence X-ray Diffraction (GIXRD) can be used to study strain at different depths within thin films. Raman spectroscopy can be used to investigate the vibrational modes of perovskites, which can be affected by strain. Changes in Raman peak positions and intensities can indicate the presence and magnitude of strain. EBSD is a technique that uses electron beams to analyze the crystallographic orientation of materials. It can be used to map strain fields within perovskite materials at the microscale. TEM can provide high-resolution images of the microstructure of perovskites, including grain boundaries and defects. TEM can also be used to measure strain at the nanoscale by analyzing the lattice fringes. AFM can be used to characterize the surface morphology and topography of perovskite films. SEM can be used to examine the morphology and grain boundaries of perovskite materials. DFT can be used to simulate the effects of strain on the electronic and optical properties of perovskite

**Strain Engineering Modulation Strategies**

***1. Compositional Tuning***

Adjusting or tuning the chemical composition of the precursor perovskite material, such as introducing other ions like Cs and Cl, can control lattice parameters and reduce microstrain. The added ions could be either in A position or halide position (X). In this scenario, the A site cations would have lower stability because of their larger or smaller ion sizes, and consequently stability could be improved by introducing additive species which crosslink between grains in precursors would enhance the stability.

***2. Film Formation Control***

Thin-film deposition techniques such as annealing or solvent engineering can be optimized to manage crystallization and reduce microstrain. When mismatch occurs if the coefficient of thermal expansions (CTE) of perovskite and the attached substrate layer are different, the annealing step can be improved by applying the perovskite layer on the substrate at room temperature using amine to lower tensile strain induced by annealing.

***3. Additive Engineering***

Introducing additives that can modify the perovskite's crystal structure and relieve or induce specific strain states. Additives can include dopants, solvents, or facets.

***4. Interface Engineering***

Interfaces between perovskite layers and other materials need to be optimized to minimize lattice mismatches induced by the difference of coefficient of thermal expansion (CTE) between layers and microstrain.

**Compositional Engineering**

1. **Modifying the A-site cation:**

Replacing methylammonium (MA) with other cations like formamidinium (FA) or cesium (Cs) can improve stability and tune the bandgap.

For example, incorporating FA into the perovskite structure can lead to a more stable and efficient material.

1. **Modifying the B-site cation:**

While lead (Pb) is commonly used, exploring other B-site cations like tin (Sn) or germanium (Ge) can lead to lead-free perovskites, addressing toxicity concerns.

Mixing different B-site cations can also help tune the bandgap and improve stability.

1. **Modifying the X-site anion:**

Using mixed halides (e.g., iodine and bromine) can help stabilize the perovskite phase and improve its performance.

The Pb-Br bond is stronger than the Pb-I bond, making bromine-containing perovskites more stable.

1. **Tuning the Perovskite Composition:**

By adjusting the ratios of different cations and anions, researchers can optimize the perovskite material for specific applications. For example, incorporating MAPbBr3 into FAPbI3 stabilizes the perovskite phase and improves power conversion efficiency.

**Examples of Compositional Engineering**

1. ***FA1-xMAxPb(I1-yBry)3:***

This composition, where FA and MA are mixed cations and I and Br are mixed anions, is a common example of compositional engineering used to improve stability and efficiency.

1. ***Guanidinium iodide (GuI) and 5-amino valeric acid iodide (5-AVAI):***

These compounds are used to enhance thermal and moisture stability of perovskite solar cells by modifying the perovskite composition and surface passivation.

1. ***Rb and Br in Perovskite Absorber Layer:***

Using Rb and decreasing the Br ratio in the perovskite absorber layer can suppress the growth of PbI2 and prevent unwanted RbBr-based aggregations, leading to improved thermal stability.

**References**

Almeida, M.A.P. and Maciel, A.P. (2018) Optical spectroscopy and its applications in inorganic materials. In: Handbook of materials characterization, Cham: Springer, pp. 293-315

Amat, A., et al. (2014) Cation-induced band-gap tuning in organohalide perovskites: Interplay of spin-orbit coupling and octahedra tilting, Nano Lett., 14(6), 3608–3616, DOI:10.1021/NL5012992/SUPPL\_FILE/NL5012992\_SI\_001.PDF.

Aydin, E., et al. (2024) Pathways toward commercial perovskite/silicon tandem photovoltaics, Science, 383(6679) DOI:10.1126/science.adh3849.

Balanov, V., Peräntie, J., Palosaari, J., Yadav, S. and Bai, Y. (2025) Study on Influence of AC Poling on Bulk Photovoltaic Effect in Pb(Mg1/3Nb2/3)O3-PbTiO3 Single Crystals, Advanced Electronic Materials, 11: 2570009, <https://doi.org/10.1002/aelm.202570009>

Bellini, Emiliano (2025W) PV Magazine, Indoor transition metal dichalcogenide solar cells may reach 36.5% efficiency,

<https://www.pv-magazine.com/2025/03/19/indoor-transition-metal-dichalcogenide-solar-cells-may-reach-36-5-efficiency/?utm_source=Global+%7C+Newsletter&utm_campaign=2b2339fc7f-dailynl_gl&utm_medium=email&utm_term=0_6916ce32b6-2b2339fc7f-160603208>

Boro, B., Porwal, S., and Kumar, D., et al. (2022) Perovskite Solar Cells: Assessment of the Materials, Efficiency, and Stability, Catalysis Research, volume 2, issue 4, <https://doi.org/10.21926/cr.2204033>

Braly, I.L., deQuilettes, D.W., Pazos-Outón, L.M., et al. (2018) Hybrid perovskite films approaching the radiative limit with over 90% photoluminescence quantum efficiency, Nat. Photonics, 12 (2018), p. 355

Brenner, T.M., et al. (2016) Hybrid organic - Inorganic perovskites: Low-cost semiconductors with intriguing charge-transport properties, Nat. Rev. Mater., 1 (1), p. 15007

Conibeer, G., Green, M., Corkish, R., et al. (2006) Silicon nanostructures for third generation photovoltaic cells, Thin Solid Films, 511-512, pp. 654.

deQuilettes, D.W., Yoo, J.J., Brenes, R. et al. (2024) Reduced recombination via tunable surface fields in perovskite thin films. Nature Energy 9, 457–466, <https://doi.org/10.1038/s41560-024-01470-5>

Elumalai, N.K. and Uddin, A. (2016) Hysteresis in organic-inorganic hybrid perovskite solar cells, Sol. Energy Mater. Sol. Cells, 157, 476–509, DOI:10.1016/J.SOLMAT.2016.06.025.

Eperon, G.E., Stranks, S.D., Menelaou, C., et al. (2014) Formamidinium lead trihalide: a broadly tunable perovskite for efficient planar heterojunction solar cells, Energy Environ. Sci., 7(3), 982–988, 10.1039/C3EE43822H.

Filip, M.R., Eperon, G.E., Snaith, H.J., and Giustino, F. (2014) Steric engineering of metal-halide perovskites with tunable optical band gaps, Nat. Commun., 5(1), 1–9, DOI:10.1038/ncomms6757.

Fujiwara, H., Kato, M., Tamakoshi, M., Miyadera, T., and Chikamatsu, M. (2018A) Optical Characteristics and Operational Principles of Hybrid Perovskite Solar Cells, Phys. Status Solidi, 215(12), 1700730, DOI:10.1002/PSSA.201700730.

Fujiwara, H., Kato, M., Tamakoshi, M., Miyadera, T. and Chikamatsu, M. (2018B) Optical Characteristics and Operational Principles of Hybrid Perovskite Solar Cells, Phys. Status Solidi, 215(12), 1700730, DOI:10.1002/PSSA.201700730.

G2V, What Are The Advantages And Disadvantages Of Perovskite Solar Cells? <https://g2voptics.com/advantages-of-perovskite-solar-cells/>

Garcia, D. (2024) Eco News. The new material that will multiply the power of solar panels: we use it every day and did not know its potential. <https://www.ecoticias.com/en/perovskite-silicon-solar-panels/397/>

Goetzberger, A., Knobloch, J., and Voss, B. (1998) Crystalline Silicon Solar Cells, Wiley, p. , p. 237, [Online], available, <https://www.wiley.com/en-us/Crystalline+Silicon+Solar+Cells-p-9780471971443>

Green, M.A. (2003) Third Generation Photovoltaics, Springer-Verlag Berlin and Heidelberg,

Germany.

Green, M.A., Ho-Baillie, A., and Snaith, H.J. (2014) The emergence of perovskite solar cells, Nat. Photonics, 8(7), 506–514, DOI:10.1038/nphoton.2014.134.

Grote, C. and Berger, R.F. (2015) Strain Tuning of Tin-Halide and Lead-Halide Perovskites: A First-Principles Atomic and Electronic Structure Study, J. Phys. Chem. C, 119(40), 22832–22837, DOI:10.1021/ACS.JPCC.5B07446/SUPPL\_FILE/JP5B07446\_SI\_001.PDF.

Haq, M.A., Saiduzzaman, M., Asif, T.I., et al. (2021) Ultra-violet to visible band gap engineering of cubic halide KCaCl3 perovskite under pressure for optoelectronic applications: insights from DFT, RSC Adv., 11(58), 36367–36378, 10.1039/D1RA06430D.

Haug, A. (1979) Non-radiative recombination of electron-hole drops by means of phonon-assisted Auger recombination, J. Lumin., 20(2), 173–177, DOI:10.1016/0022-2313(79)90048-6.

Hossain, M.I., et al. (2021) Near field control for enhanced photovoltaic performance and photostability in perovskite solar cells, Nano Energy, 89, 106388, DOI:10.1016/J.NANOEN.2021.106388.

Hutter, E.M., et al. (2016) Direct–indirect character of the bandgap in methylammonium lead iodide perovskite, Nat. Mater., 16(1), 115–120, DOI:10.1038/nmat4765.

Jiang, S., Wang, R., Li, M., et al. (2024B) Synergistic electrical and light management enables efficient monolithic inorganic perovskite/organic tandem solar cells with over 24% efficiency, Energy Environ. Sci., 17(1), 219–226, 10.1039/D3EE02940A.

Jung, S.K., Park, N.G., and Lee, J.W. (2023) Light management in perovskite solar cells, Mater. Today Energy, 37, 101401, DOI:10.1016/J.MTENER.2023.101401.

Kangsabanik, J., Svendsen, M.K., Taghizadeh, A., et al. (2022) Indirect Band Gap Semiconductors for Thin-Film Photovoltaics: High-Throughput Calculation of Phonon-Assisted Absorption, J. Am. Chem. Soc., 144(43), 19872–19883, DOI:10.1021/JACS.2C07567/SUPPL\_FILE/JA2C07567\_SI\_001.PDF.

Kim, J., Lee, S.C., Lee, S.H., and Hong, K.H. (2015A) Importance of orbital interactions in determining electronic band structures of organo-lead iodide, J. Phys. Chem. C, 119(9), 4627–4634, DOI:10.1021/JP5126365/SUPPL\_FILE/JP5126365\_SI\_001.PDF.

Kim, J., Lee, S.H., Chung, C.H., and Hong, K.H. (2016A) Systematic analysis of the unique band gap modulation of mixed halide perovskites, Phys. Chem. Chem. Phys., 18(6), 4423–4428, 10.1039/C5CP05982H.

Kim, J., Kim, H., Teridi, M. et al. (2016B) Bandgap tuning of mixed organic cation utilizing chemical vapor deposition process. Sci Rep 6, 37378, <https://doi.org/10.1038/srep37378>

Kong, L., et al. (2016) Simultaneous band-gap narrowing and carrier-lifetime prolongation of organic-inorganic trihalide perovskites, Proc. Natl. Acad. Sci. U. S. A., 113(32), 8910–8915, DOI:10.1073/PNAS.1609030113/SUPPL\_FILE/PNAS.1609030113.SAPP.PDF.

Kulkarni, S.A., Baikie, T., Boix, P.P., et al. (2014) Band-gap tuning of lead halide perovskites using a sequential deposition process, J. Mater. Chem. A, 2, 9221-9225, <https://pubs.rsc.org/en/content/articlehtml/2014/ta/c4ta00435c>

Landsberg, P.T., and Baruch, P. (1989) “The thermodynamics of the conversion of radiation

energy for photovoltaics”, Journal of Physics A: Mathematical and General, 22, pp. 1911-

1926.

Lehner, A.J., et al. (2015) Crystal and Electronic Structures of Complex Bismuth Iodides A3Bi2I9 (A = K, Rb, Cs) Related to Perovskite: Aiding the Rational Design of Photovoltaics, Chem. Mater., 27(20), 7137–7148, DOI:10.1021/ACS.CHEMMATER.5B03147/SUPPL\_FILE/CM5B03147\_SI\_001.PDF.

Lei, Y., Li, Y., and Jin, Z. (2022) Photon energy loss and management in perovskite solar cells, Energy Rev., 1(1), 100003, DOI:10.1016/J.ENREV.2022.100003.

Lewis, Michelle (2024) Electrek. MIT just released directions for commercializing perovskite solar cells. <https://electrek.co/2024/02/28/mit-just-released-directions-for-commercializing-perovskite-solar-cells/>

Liang, D. and Bowers, J.E. (2010) Recent progress in lasers on silicon, Nat. Photonics, 4(8), 511–517, DOI:10.1038/nphoton.2010.167.

Liao, W., Zhao, D., Yu, Y., et al. (2016A) Fabrication of efficient low-bandgap perovskite solar cells by combining formamidinium tin iodide with methylammonium lead iodide, J Am Chem Soc., 138, 12360-12363

Liu, G., Kong, L., Yang, W., and Kwang Mao, H. (2019A) Pressure engineering of photovoltaic perovskites, Mater. Today, 27, 91–106, DOI:10.1016/J.MATTOD.2019.02.016.

Lu, H., Krishna, A., Zakeeruddin, S., Grätzel, M., and Hagfeldt, A. (2020). Compositional and Interface Engineering of Organic-Inorganic Lead Halide Perovskite Solar Cells. iScience. 101359,

<https://www.researchgate.net/publication/342861512_Compositional_and_Interface_Engineering_of_Organic-Inorganic_Lead_Halide_Perovskite_Solar_Cells>

Malyi, O.I. and Acosta, C.M. (2020) Amorphization of Indirect Band Gap Semiconductors to Tune Their Optoelectronic Properties, J. Phys. Chem. C, 124(27), 14432–14438, DOI:10.1021/ACS.JPCC.0C02332/SUPPL\_FILE/JP0C02332\_SI\_001.PDF.

Meillaud, F., Shah, A., Droz, C., Vallat-Sauvain, E., and Miazza, C. (2006) Efficiency limits for single-junction and tandem solar cells, Sol. Energy Mater. Sol. Cells, 2006, 90 , 2952 —2959

Miao, Y., et al. (2021) Construction of efficient perovskite solar cell through small-molecule synergistically assisted surface defect passivation and fluorescence resonance energy transfer, Chem. Eng. J., 426, 131358, DOI:10.1016/J.CEJ.2021.131358.

Mirage News (2025) Strain Trick Boosts Perovskite Solar Cell Efficiency,

<https://www.miragenews.com/strain-trick-boosts-perovskite-solar-cell-1441513/>

Monllor-Satoca, D., Gómez, R., González-Hidalgo, M. and Salvador, P. (2007) The ‘Direct–Indirect’ model: An alternative kinetic approach in heterogeneous photocatalysis based on the degree of interaction of dissolved pollutant species with the semiconductor surface, Catal. Today, 129(1–2), 247–255, DOI:10.1016/J.CATTOD.2007.08.002.

Nitta, F.U., Nazif, K.N., Pop, E. (2025) Transition metal dichalcogenide solar cells for indoor energy harvesting, Device, 100723, <https://doi.org/10.1016/j.device.2025.100723>

Noh, J.H., Im, S.M., Heo, J.H., Mandal, T.N., and Il Seok, S. (2013) Chemical management for colorful, efficient, and stable inorganic-organic hybrid nanostructured solar cells, Nano Lett., 13(4), 1764–1769, DOI:10.1021/NL400349B/SUPPL\_FILE/NL400349B\_SI\_001.PDF.

Ou, Q., et al. (2019) Band structure engineering in metal halide perovskite nanostructures for optoelectronic applications, Nano Mater. Sci., 1(4), 268–287, DOI:10.1016/J.NANOMS.2019.10.004.

Parrott, E.S., et al. (2016) Effect of Structural Phase Transition on Charge-Carrier Lifetimes and Defects in CH3NH3SnI3 Perovskite, J. Phys. Chem. Lett., 7 (7), pp. 1321-1326

Peplow, Mark (2023) A new kind of solar cell is coming: is it the future of green energy? Nature, <https://www.nature.com/articles/d41586-023-03714-y>

Pilkuhin, M.H. (1979) Non-radiative recombination and luminescence in silicon, J. Lumin., 18–19(PART 1), 81–87, DOI:10.1016/0022-2313(79)90078-4.

Prakash, J., et al. (2018) Progress in tailoring perovskite based solar cells through compositional engineering: Materials properties, photovoltaic performance and critical issues, Mater. Today Energy, 9, 440–486, DOI:10.1016/J.MTENER.2018.07.003.

Priyanka, E. and Muchahary, D. (2024) Performance improvement of perovskite/CIGS tandem solar cell using barium stannate charge transport layer and achieving PCE of 39 % numerically, Sol. Energy, 267, 112218, DOI:10.1016/J.SOLENER.2023.112218.

Saliba, M., et al. (2016) Cesium-containing triple cation perovskite solar cells: Improved stability, reproducibility and high efficiency, Energy Environ. Sci., 9(6), 1989–1997, 10.1039/C5EE03874J.

Schaadt, D.M., Feng, B., and Yu, E.T., 2005. “Enhanced semiconductor optical absorption

via surface plasmon excitation in metal nanoparticles”, Applied Physics Letters, 86, p.

063106.

Shaikh, Kaif (2025) Interesting Engineering, 35% power boost: New solar cell technology achieves significant electric output,

<https://interestingengineering.com/energy/solar-cell-more-electric-output>

Shi, D., et al. (2015) Low trap-state density and long carrier diffusion in organolead trihalide perovskite single crystals, Science, 347 (6221), pp. 519-522

Shockley W., and Queisser, H.J. (1961) “Detailed balance limit of efficiency of p-n junction

solar cells”, Applied Physics Letters, 32, pp. 510-519.

Solanki, C.S., and Beaucarne, G. (2007) Advanced Solar Cell Concepts, Energy for Sustainable Development, Volume 11, Issue 3, Pages 17-23, <https://www.sciencedirect.com/science/article/abs/pii/S0973082608605736>

Son, D.Y., et al. (2016) Self-formed grain boundary healing layer for highly efficient CH3NH3PbI3 perovskite solar cells, Nat. Energy, 1(7), 1–8, DOI:10.1038/nenergy.2016.81.

Song, Z., Chen, C., Li, C., et al. (2019) Wide-bandgap, low-bandgap, and tandem perovskite solar cells, Semicond Sci Technol., 34, 093001

Stenzel, O., Stendal, A., Voigtsberger, K., and von Borczyskowski, C., 1995. “Enhancement

of the photovoltaic conversion efficiency of copper phthalocyanine thin film devices by incorporation of metal clusters”, Solar Energy Materials and Solar Cells, 37, pp. 337-348.

Sutherland, B.R. and Sargent. E.H. (2016) Perovskite photonic sources, Nat. Photonics, 10, p. 295

Tanaka, K., Takahashi, T., Ban, T., et al. (2003) Comparative study on the excitons in lead-halide-based perovskite-type crystals CH3NH3PbBr3 CH3NH3PbI3, Solid State Commun, 127, 619– 623

Tao, Xucheng, "Strain engineering in perovskite" (2022). Mechanical Engineering and Materials Science Independent Study. 171. <https://openscholarship.wustl.edu/mems500/171>

Welte, A., Waldauf, C., Brabec, C., and Wellmann, P.J. (2008) Application of optical absorbance for the investigation of electronic and structural properties of sol–gel processed TiO2 films, Thin Solid Films, 516(20), 7256–7259, DOI:10.1016/J.TSF.2007.12.025.

Xia, Y., et al. (2023) Organic-Inorganic Hybrid Quasi-2d Perovskites Incorporated with Fluorinated Additive for Efficient and Stable Four-Terminal Tandem Solar Cells, Energy Mater., 3(1), 300004, DOI:10.20517/energymater.2022.55.

Xing, J., et al. (2018) Color-stable highly luminescent sky-blue perovskite light-emitting diodes, Nat. Commun., 9(1), 1–8, DOI:10.1038/s41467-018-05909-8.

Xu, J., Castriotta, L.A., Di Carlo, A., and Brown, T.M. (2024) Air-Stable Lead-Free Antimony-Based Perovskite Inspired Solar Cells and Modules, ACS Energy Lett., 9(2), 671–678, DOI:10.1021/ACSENERGYLETT.3C02409.

Yang, W.S., Noh, J.H., Jeon, N.J., et al., (2015) High-performance photovoltaic perovskite layers fabricated through intramolecular exchange, Science, 348, 1234.

Yang, C., Hu, W., Liu, J. et al. (2024) Achievements, challenges, and future prospects for industrialization of perovskite solar cells. Light Sci Appl 13, 227, <https://doi.org/10.1038/s41377-024-01461-x>

Zanatta, A.R. (2022) The Shockley–Queisser limit and the conversion efficiency of silicon-based solar cells, Results Opt., 9, 100320, DOI:10.1016/J.RIO.2022.100320.

Zheng, L., Wei, M., Eickemeyer, F.T., et al. (2025) Strain-induced rubidium incorporation into wide-bandgap perovskites reduces photovoltage loss. Science.;388(6742):88-95

Zientara, Ben (2025) Solar Reviews, Perovskite solar cells: why they’re the future of solar power,

<https://www.solarreviews.com/blog/are-perovskite-solar-cells-the-future-of-solar-power>

1. Solar Mag (2022) Perovskite Solar Cells: An In-Depth Guide + Comparisons With Other Techs,

   <https://solarmagazine.com/solar-panels/perovskite-solar-cells/#:~:text=Perovskite%20silicon%20tandem%20solar%20cells,silicon%20(nc%2DSi)> [↑](#footnote-ref-0)
2. G2V, What Are The Advantages And Disadvantages Of Perovskite Solar Cells? <https://g2voptics.com/advantages-of-perovskite-solar-cells/> [↑](#footnote-ref-1)
3. G2V, What Are The Advantages And Disadvantages Of Perovskite Solar Cells? <https://g2voptics.com/advantages-of-perovskite-solar-cells/> [↑](#footnote-ref-2)