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Efficiency and Stability of 2-D Material-Based Perovskite Solar Cells

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Abstract
Perovskites are recognized as highly promising materials for third-generation solar cells. There are still significant difficulties that need to be addressed concerning the efficiency and stability of devices. The efficiency of perovskite solar cells (PSCs) is significantly influenced by the dynamics of charge carriers. The intricate process involves the generation, extraction, transit, and collection of charge carriers, all of which must be controlled effectively to obtain optimal performance. Two-dimensional materials (TDMs) such as graphene, transition metal dichalcogenides (e.g. MoS2, WS2), black phosphorus (BP), metal nanosheets, and two-dimensional (2D) perovskite active layers are being widely studied for their high carrier mobility and adjustable work function properties, which significantly influence the charge carrier dynamics of perovskite solar cells. Significant progress has been made for TDMs-based PSCs so far. This paper discusses the latest advancements in utilizing TDMs like as graphene, graphdiyne, transition metal dichalcogenides, BP, and others as electrodes, hole transporting layers, electron transporting layers, and buffer layers in PSCs. 2D perovskites are discussed as efficient absorber materials in PSCs. This discussion focuses on how TDMs and 2D perovskites impact the movement of electric charges in PSCs to further our understanding of their light-electricity conversion processes. The PSC devices' issues are highlighted along with solutions aimed at enhancing the efficiency and stability of solar devices.

Introduction

Photovoltaic solar cells can convert energy from the sun into direct current electricity using the photovoltaic effect. Such devices have been regarded as a very promising energy generation source and attracted much attention from the academic community. [1] Several photovoltaic solar cells have helped to shape the environment of renewable sources of energy, including silicon solar cells, III-V solar cells, quantum dot-sensitized solar cells, dye-sensitized solar cells, organic solar cells and perovskite solar cells (PSCs). [2] Crystalline silicon is non-toxic, readily available, and enables the production of solar cells that can achieve conversion efficiencies of up to 27% with minimal degradation. [3] Due to these factors, it has consistently maintained its position as the market leader over an extended period of time. [4-5] Yet, this advanced technology is limited by inherent disadvantages, including high temperature and energy-intensive production methods, and a substantial worldwide need for silicon. [6] The efficiency of crystalline solar cells relies heavily on their uninterrupted structure with minimal grain boundaries to enhance the mobility of photo-generated carriers. The primary commercial incentive for creating highly efficient photovoltaic solar cells is to lower production expenses and generate top-notch semiconductors. PSCs have rapidly emerged as one such candidate. [7] The development of PSCs is on its way to challenging the dominance of polycrystalline silicon and other thin film technologies. High power conversion efficiencies can be achieved by simple low cost processing. The term “perovskite” is used to describe compounds with the formula ABO3, in which A denotes the larger atom (cuboctahedral coordination), B denotes the smaller atoms. [8] In general, A and B are two cations while O is an anion that bonds to both. The coordination may deviate from ideal due to the differences in the atomic radii of the constituents. [9-15] This deviation from ideality is defined by the Goldschmidt tolerance factor (t).

The Goldschmidt tolerance factor can predict the stability and distortion of the crystal structure of ABO3 perovskite materials and is defined by the expression

$$t = \frac{r_A + r_O}{\sqrt{2}(r_B + r_0)}$$

where r_A, r_B, and r_O are the ionic radii of A, B, and O, respectively.

The cubic structure can cause distortions, leading to layered two-dimensional (2D) perovskites. The Ruddlesden-Popper (RP) phase is a 2D perovskite structure with interlayered 2D slabs. As n increases, structural gradients from 2D to 3D perovskites coexist. 2D perovskites have attracted attention due to their advantageous 2D shape for charge carrier migration and intrinsic photovoltaic properties. They can be assembled into uniform, ultrathin flexible films with highly oriented microstructures. Unlike 3D perovskites, 2D perovskites have tunable photoelectric properties and excellent environmental stability. [17-21]

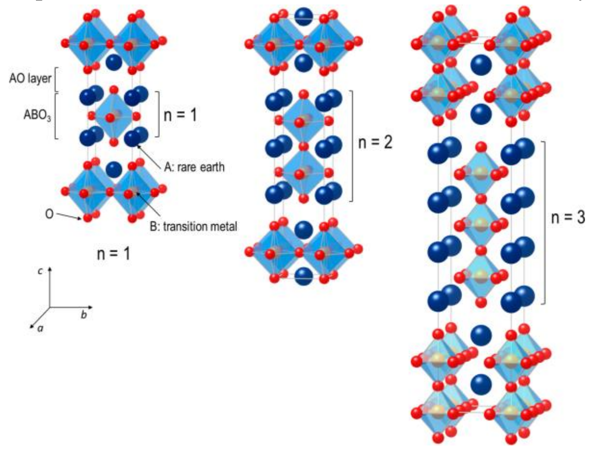

Figure 1. The ideal Ruddlesden–Popper-type perovskite structure.

Organic-inorganic metal halide perovskites, like MAPbI3, are used in solar cells for efficiencies of 3.8%. In 2012, they were used in solid-state meso-superstructured photocatalysts (PSCs), achieving a power conversion efficiency of 9.7%. [18-23] To date, numerous TDMs have been reported, and they can be categorized into groups based on their structural similarities:

1. materials with atomic layers arranged in hexagonal honeycomb lattices, such as graphene, borophene, germanene, hexagonal-boron nitride (h-BN), and black phosphorus (BP);
2. transition metal dichalcogenide with a general stoichiometric formula of MX2 (where M represents the transition metal and X represents the chalcogen, e.g., MoS2, MoSe2 and WS2); and
3. metal oxide nanosheets/nanoplates, such as titania nanosheets and ZnO nanoplates.

2. Experimental Methodology

The preparation of TDMs by exfoliation is cost-efficient and versatile, as it can be combined with other chemical treatments to produce various functionalized TDMs. [24-27] Mechanical exfoliation is widely used to prepare single or few layered TDMs by applying mechanical forces to solutions of layered materials via stirring, shaking, or ultra-sonication. Surfactants are commonly employed to reduce van der Waals interactions and keep the exfoliated products suspended in the solvent. [28-30] Chemical exfoliation methods, such as ion intercalation and solvent-based exfoliation, are employed to produce TDMs of one or a few layers. [31] Two-dimensional perovskites have a layered structure, with the most commonly reported layered 2D perovskite having an orientation of L2(ABX3)n-1BX4. These perovskite compounds exhibit attractive optical properties due to their stable excitons and large binding energy. [32] Liquid phase methods using organic alkyl ammonia derivatives are commonly used for synthesizing perovskites with different morphologies, including perovskite nanosheets and nanoplatelets.

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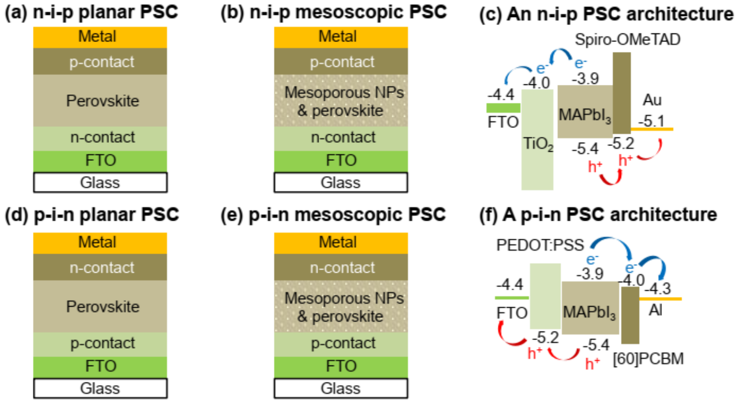

Figure 2. Solid-state device architectures of n-i-p and p-i-n planar, and energy band diagram architecture of FTO/TiO2/MAPbI3/Spiro-OMeTAD/Au.

Vapor phase methods transform perovskite precursors into gas phase through sublimation, evaporation, or decomposition, resulting in the condensed vapor. [33] These methods offer conformal and controllable thin film growth and enable the vapor phase epitaxial growth of perovskites with mismatched lattice constants. [34-36] They synthesize more uniform films over larger areas with improved crystallinity and reduced impurities. The performance of TDMs and 2D perovskites in photo-switched solar cells (PSCs) is significantly impacted by their optical and electronic properties. The general experimental setup of a CVD experiment for preparing two-dimensional graphene consists of a furnace, a quartz chamber, a control system, and mass flow controllers (MFC) for reactant gases.

Result and Discussion

Transparent electrodes are essential for high-performance photovoltaic solar cells (PSCs) as they should be highly conductive, inexpensive, stable, and effective charge collectors. Traditional transparent electrode materials like indium tin oxide (ITO) and PEDOT:PSS are fragile and hydroscopic, leading to the destruction of perovskite layers. [37] Graphene is a promising material for PSC electrodes due to its earth abundant carbon composition, excellent electrical and optical properties, and mechanical toughness. Large-area graphene grown by CVD has been used as a transparent electrode in PSCs, showing high optical transmission below the perovskite energy bands, leading to superior charge collection efficiency. [38-39] However, the transfer step for depositing graphene electrodes into PSC devices has lower reproducibility, which can significantly affect the conductivity of graphene electrodes. A more consistent graphene transfer method is required to improve reproducibility and justify the use of highly conductive graphene electrodes in PSC devices. [40]

Semi-transparent PSCs were first reported by laminating stacked multi-layer graphene prepared by CVD as the top transparent electrode. Poly(3-hexylthiophene) (P3HT) was found to be a good candidate as the supporting polymer of graphene electrode. Graphene electrodes are promising for PSCs due to their high light transmittance and ductility, but sheet resistance and fracturing resistance make them challenging to use in PSCs. [41] Doping with materials like P3HT and MoO3 has proven effective in improving the performance of graphene-based PSC devices, optimizing the work function of graphene, and minimizing the energy barrier between the electrode and charge transport layers. [42]

Phosphorene (BP) is a promising 2D nanomaterial due to its electronic and optoelectronic properties. It is flexible, stable, and can be mechanically exfoliated. BP-based PSCs have a PCE of 7.88%, 4% higher than HTL-free devices. Metal oxide nanosheet materials are also investigated for use as HTLs in PSCs due to their large specific surface area. [43] PSC device performance is governed by electronic energy levels, charge carrier mobility, effective charge extraction from the perovskite layer, and charge collection by electrodes. 2D graphene is chosen as a buffer layer in photovoltaic solar cells (PSCs) due to its high band gap, transparency, and mesoporous structure. Carbon nanostructures in PSCs can improve cell stability due to their hydrophobicity. 2D perovskite active layer materials in solar cells exhibit excellent photoelectric conversion efficiencies and maintain light absorption properties. [44] The layered 2D

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perovskite structure offers greater tunability at the molecular level for optimizing optical and electrical properties. Long-term device stability remains a challenge in solar cells due to several reaction pathways involving water, oxygen, light, acid, and heat. An interfacial buffer layer can improve the stability of PSCs in the presence of moisture and oxygen.

Conclusions

The diffusion of molecular oxygen can activate the formation of peroxide or superoxide compounds that attack and degrade active layers in photovoltaic (PSC) devices. Long-term stability of PSCs in the presence of moisture and oxygen can be improved by an interfacial buffer layer, which avoids direct contact between perovskite and moisture. Two-dimensional graphene-related materials are known for their thermal, mechanical, and chemical stability, and can be easily processed into uniform ultrathin optically transparent layers. PEDOT:PSS is typically used as the HTL in PSCs, which is acidic and hygroscopic in nature, facilitating the decomposition of active layers. 2D perovskites have been recognized as improving the stability of PSCs, but the underlying mechanism remains unclear. The hydrophobic properties of long organic side groups in the 2D perovskite structure prevent direct contact between water and perovskite layer. Despite their superior stability, the efficiency of 2D-based PSCs is unsatisfactory due to suppressed out-of-plane charge transport by organic cations in 2D perovskites.

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Conflict of Interest Statement

The authors conducted ethical and transparent research, demonstrating the importance of ethical practices in scientific research.

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