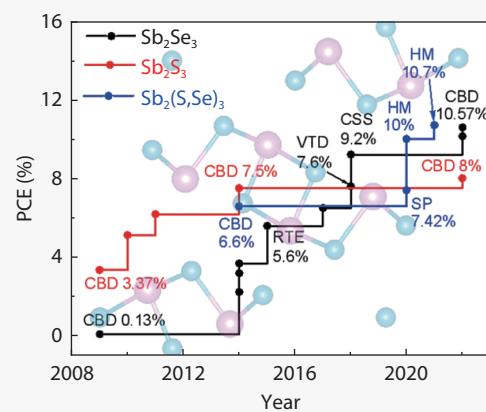


Low-dimensional antimony selenosulfide as an emerging material for solar cell applications

Lijian Zhang^{1,2}, Chunyan Wu³, Wenhao Liang^{1,2} and Tao Chen^{1,2*} 

Antimony chalcogenides (Sb_2X_3), including Sb_2S_3 , Sb_2Se_3 , and the alloy-type $Sb_2(S,Se)_3$, have been considered as a promising absorber materials for photovoltaic applications. Owing to its unique quasi-one-dimensional crystal structure, it displays distinct defect and carrier transport properties and requires special material synthesis strategy compared with the traditional three-dimensional crystal structure semiconductor materials. Recent studies on this class of materials have generated new understandings in film fabrication, defect characteristics and passivation, interfacial engineering, and efficiency improvement. With these efforts, the power conversion efficiency of the solar cell device has been increased from below 3% to 10.7% over the past 10 years. This efficiency achievement suggests that Sb_2X_3 possesses great potential for practical applications with further efficiency enhancement. This perspective article presents the critical development in the Sb_2X_3 materials and solar cells in recent years, including the unique crystal structure for solar cells, the preparation method for obtaining high-quality Sb_2X_3 films, and the discovery and passivation of unusual and complex defects. Finally, we propose several strategies for future efficiency improvement.



With the rapid increase of global energy consumption, the urgent demand for renewable energy is growing fast. Solar cell directly absorbs sunlight and converts it into electricity, which is considered as one of the most important green energy conversion technologies. Among photovoltaic devices, inorganic thin film solar cells do not require ultrahigh-purity absorber materials which would potentially reduce the fabrication cost. It is also found that thin film solar cells are suitable for some special applications such as flexible and light-weight portable devices, owing to the versatile properties.^[1] For instance, the CdTe solar cells have been successfully applied in the building-integrated photovoltaics (BIPV); Cu(In,Ga)(S,Se)₂ (CIGS) solar cells are suitable for stable flexible device with either metal foil or transparent substrate.^[2-3] However, owing to the scarcity of In and

Ga in CIGS, the toxicity of Cd in CdTe, researchers have put great efforts in exploring new and green metal chalcogenide light-harvesting materials, with particular interest in those with the high stability, earth abundance, and environmental-friendly constituents.^[4] In this regard, antimony chalcogenides (Sb_2X_3), including Sb_2S_3 , Sb_2Se_3 , and the alloy-type $Sb_2(S,Se)_3$, have recently been manifested to be a promising light-absorbing material for the next generation thin film solar cells.^[5-8]

Sb_2X_3 is chemically stable and composed of abundant elements which are not included in the lists of highly toxic or hazardous materials by Chinese, American as well as European Union regulation authorities.^[9] Therefore, it is considered as a green light-absorbing material. Additionally, Sb_2X_3 exhibits high light absorption coefficient ($>10^5 \text{ cm}^{-1}$ in visible region), indicating that the application as absorber layer at hundreds of nanometers can harvest sufficient sunlight. Furthermore, Sb_2S_3 and Sb_2Se_3 possess identical crystal structure and the atomic ratio of S/Se can be tuned in continuous manner, which enables the bandgap tunable in the range of 1.1–1.7 eV.^[8, 10] This bandgap value falls into the optimal range for solar cell applications according to Shockley-Queisser detailed-balance efficiency theory (Figure 1a),^[8] suggesting that the theoretical power conversion efficiency (PCE) of Sb_2X_3 can reach 32%. What's more, Sb_2X_3 possesses a unique quasi-one-dimensional (Q1D) crystal structure, resulting in

¹ Hefei National Research Center for Physical Sciences at the Microscale, CAS Key Laboratory of Materials for Energy Conversion, Department of Materials Science and Engineering, University of Science and Technology of China, Hefei 230026, China

² Institute of Energy, Hefei Comprehensive National Science Centre, Hefei 230001, China

³ Laboratory of Advanced Nano-Optoelectronic Materials and Devices, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Science, Ningbo 315201, China

* Corresponding author, E-mail: tchenmse@ustc.edu.cn

Received 8 December 2022; Accepted 24 July 2023; Published online

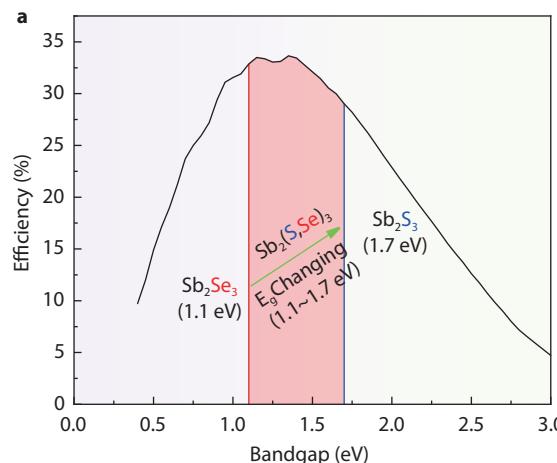


Fig. 1 **a** Theoretical Shockley-Queisser detailed-balance efficiency limit as a function of bandgap.^[18] Copyright 2016, Science. **b** Record efficiencies of Sb_2X_3 solar cells. Note: CBD stands for chemical bath deposition; RTE stands for rapid thermal evaporation; VTD stands for vapor transport deposition; CSS stands for close spaced sublimation; SP stands for spin-coating method; HM stands for hydrothermal method.

the unique carrier transport properties. This unique crystal structure is also believed to tolerate certain bending which render the potential applications in flexible device. Owing to above unique properties, during the past decade, Sb_2X_3 solar cells have experienced a significant increase in PCE from an initial value of below 3% to the record of 10.7% in 2021.^[11] Figure 1b exhibits the significant progress of Sb_2X_3 solar cells in PCE.^[1, 12-15] The highest reported PCEs of Sb_2S_3 , Sb_2Se_3 , and $\text{Sb}_2(\text{S},\text{Se})_3$ are 8.0%, 10.57%, and 10.7%, respectively.^[11, 16-17] The corresponding method for the synthesis of antimony based absorber films are also included (Figure 1b).

This rapid increase in PCE confirms that the Sb_2X_3 solar cells have a promising application prospect. This perspective focuses on the both basic understanding of the materials and significant progress on the Sb_2X_3 solar cells, which is divided into four sections: (i) the unique crystal structure and properties, (ii) the deposition methods for high-quality thin film, (iii) defect characterization and passivation, (iv) conclusions and outlook.

Structure determined Unique Carrier Transport and Flexibility

As for Sb_2X_3 , the most attractive feature is its Q1D structure, which is different from the widely explored photovoltaic absorber materials, such as Si, CIGS, and CdTe who possess a three-dimensional (3D) crystal structure. 3D crystal structure guarantees isotropic carrier transport, which do not require the orientation control in the film preparation. However, the multi-crystalline film usually generates dangling bonds at grain boundaries (GBs) which would act as recombination centers (Figure 2a). Therefore, post-treatment is generally required to remedy the defects.^[7] In contrast, in the case of Sb_2X_3 , $(\text{Sb}_4\text{X}_6)_n$ ribbons are covalently bonded through Sb-X bonds along [001] direction (Figure 2b). The in-plane ribbons are held together in parallel along the [010] and [100] via weak van der Waals force, forming layered sheets of Sb_2X_3 .^[7, 19] This unique Q1D crystal structure leads to the strongly anisotropic carrier transport properties: the carrier transport along the ribbon is more efficient than charge hopping between

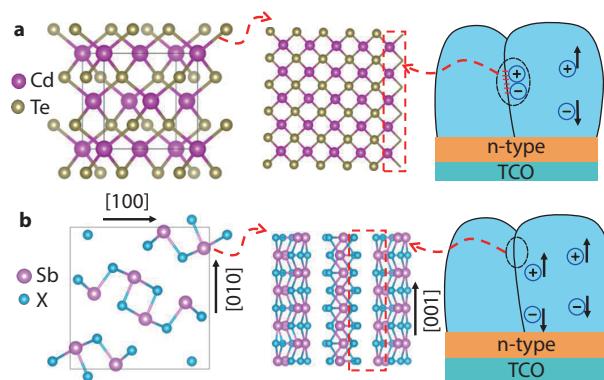
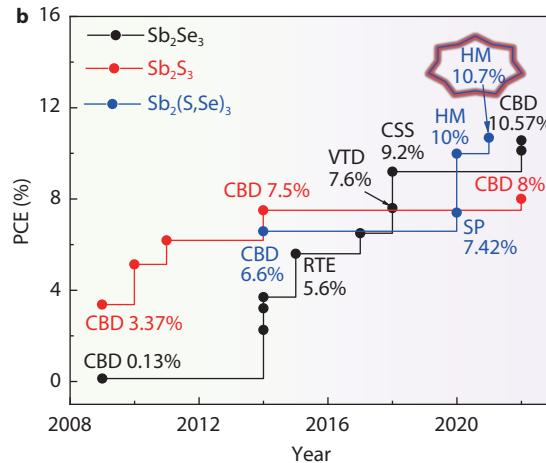


Fig. 2 Crystal structure and recombination loss at the GBs in CdTe and Sb_2Se_3 solar cells. **a** CdTe possesses a 3D crystal structure and has dangling bonds (shown as red rods) at the GBs, which act as defects that cause recombination loss of the photo-generated carriers. **b** Sb_2X_3 is composed of $(\text{Sb}_4\text{X}_6)_n$ ribbons stacked in parallel in the [001] direction. Introduce no recombination loss at the GBs once they are oriented vertically onto the substrates.^[7] Copyright 2015, Springer Nature.

ribbons. In fact, the hole mobility of [020]-, [120]- and [221]-oriented Sb_2Se_3 films was estimated as 0.69, 0.81 and 1.25 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, respectively, measured by time of flight method, confirming higher mobility along $[\text{hkl}, \text{l} \neq 0]$ orientations than that along $[\text{hkl}, \text{l} = 0]$ orientations.^[20] Additionally, the GBs parallel to c-axis are free of dangling bonds (Figure 1b).^[21] In this regard, the potential issue of bulk recombination loss through dangling bonds at the GBs can be effectively alleviated and the carrier transport efficiently in polycrystalline Sb_2X_3 if Sb_2X_3 grows along the $[\text{hkl}, \text{l} \neq 0]$ direction.

Additionally, the Q1D structure makes Sb_2X_3 has unusual deformation tolerance because of the large gap and weak interaction force between the adjacent $(\text{Sb}_4\text{X}_6)_n$ ribbons.^[22-24] It has been demonstrated that Sb_2Se_3 has a high fracture strain of 28% through the theoretical calculation research (Figure 3a).^[23] Specially, if the Sb_2Se_3 film deposited on substrate strictly along with [001] orientation, the device performance would not degrade when bent to the extreme that the frac-

ture occurs (Figure 3b).^[22] Furthermore, the material's low melting point enables it to form high-quality thin film at mild annealing temperatures (about 300~400 °C). Therefore, Sb_2Se_3 has intrinsic advantages in flexible solar cells than other conventional inorganic solar cells. Recently, flexible Sb_2Se_3 solar cells have been realized based on the substrates of Mo foils or polyimides.^[22, 25-26] Wen et al. prepared a flexible Sb_2Se_3 solar cell with an impressive PCE of 7.15%. This flexible device maintained over 90% of the initial efficiency after 1000 bending cycles with a 50° bending angle.^[26] Moreover, Li et al. demonstrated that flexible Sb_2Se_3 solar cell based on polyimide substrate showed power per-weight of 2.04 W/g which is larger than the optimal ultrathin flexible CdTe and InP solar cells and is comparable to the ultrathin CIGS flexible solar cells (Figure 3c).^[22] Owing to the excellent lightweight and bending tolerance properties of flexible Sb_2Se_3 solar cells, integrating them with the Internet of Things (IoT) as energy supply device is valuable for commercial application (Figure 3d).^[23] It is expected that flexible Sb_2X_3 solar cells can be applied in various IoT scenarios include intelligent buildings and mobile health gadgets.

Recent Achievements in Sb_2X_3 Deposition Strategies

As an emerging material for solar cell applications, the most urgent task is to improve the PCE of Sb_2X_3 solar cells. In this regard, developing novel film preparation method is one of the most effective strategies to enhance the PCE of thin film solar cells, because high-quality thin films with low density of defect and large grain size can be prepared through regulating the deposition parameters. In fact, the preparation of CIGS, CdTe, and even organic-inorganic perovskite photo-

voltaic films provides rich experiences for developing effective methods to prepare high-quality Sb_2X_3 film, while a suitable advancement is also required for the fabrication of high quality Sb_2X_3 films. Typically, chemical bath deposition, spin-coating, hydrothermal deposition, and physical vapor deposition, etc. were developed to prepare high-quality Sb_2X_3 films (Table 1).^[6, 27-29] The synthesis methods for typical Sb_2X_3 solar cells along with devise structures are summarized in Table 1. Here we mainly focus on physical vapor deposition and hydrothermal method to discuss the achievements in the Sb_2X_3 solar cells, since both have made great progresses in improving the PCE of Sb_2X_3 solar cells.

The application of Sb_2X_3 in solar cells can be dated back to 2009, in which Sb_2S_3 was used as solid-state semiconductor absorber in dye-sensitized solar cell and yielded a PCE of 3.37%.^[30] Since then, the understanding of the fundamental properties of Sb_2X_3 for solar cell applications has gradually improved, especially the carrier transport anisotropy caused by Q1D crystal structure. In this regard, the Tang group achieved the deposition of [221]-oriented Sb_2Se_3 film on a planar CdS substrate via rapid thermal evaporation (RTE), yielding a certified PCE of 5.6%.^[7, 19] This research showed that Sb_2X_3 with Q1D crystal structure offers promise as absorbers once the film is oriented suitably for transport. Additionally, this crystal structure can simultaneously sustain excellent transport along one axis and minimal recombination (owing to the benign GBs) along the orthogonal axes. Then, it has been increasingly acknowledged that the $(\text{Sb}_4\text{Se}_6)_n$ ribbons of highly [221]-oriented Sb_2Se_3 is favorable for the carriers transporting. Thus, depositing Sb_2X_3 films with preferred orientation to improve the PCE has become an important research hotspot in this field. Considering this issue, Li et al. developed a close-spaced sublimation (CSS) method to pro-

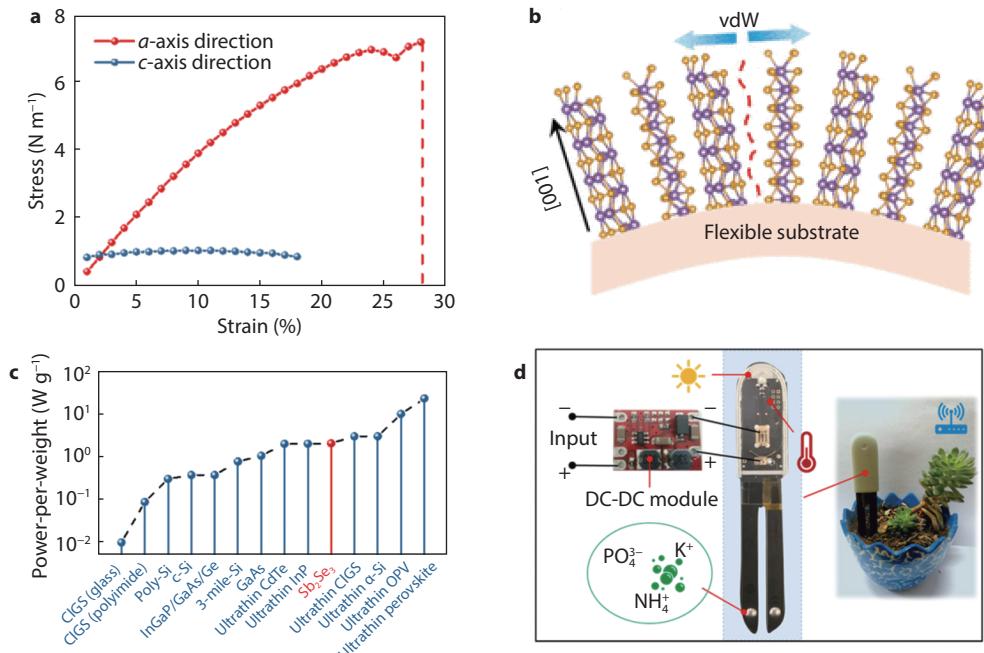


Fig. 3 **a** The calculated stress of Sb_2Se_3 film as a function of strain and **b** Large deformation tolerance for [hk0]-free orientations.^[23] Copyright 2020, American Chemical Society. **c** Power-per-weight (PPW) of the flexible Sb_2Se_3 solar cells based on polyimide substrates and the other well-developed flexible solar cells and **d** schematic diagram of the Sb_2Se_3 mini-module and the flower monitor.^[22] Copyright 2021, Elsevier.

Table 1. Typical photovoltaic performances of Sb_2X_3 solar cells reported in the literature based on absorber deposition methods, along with device structure and defect passivation approach.

Device structure	Deposition method	Passivation approach	PCE (%)	Year/Ref.
FTO/c-TiO ₂ /porous-TiO ₂ /Sb ₂ S ₃ /CuSCN/Au	Chemical bath deposition	/	3.37	2009/[30]
FTO/c-TiO ₂ /mp-TiO ₂ /Sb ₂ S ₃ /PCPDTBT/Au	Chemical bath deposition	Thioacetamide treatment	7.5	2014/[6]
FTO/c-TiO ₂ /Sb ₂ S ₃ /Au	Rapid thermal evaporation	Cu doping	4.61	2019/[31]
FTO/CdS/Sb ₂ S ₃ /Spiro-OMeTAD/Au	Thermal evaporation	In situ sulfization	6.2	2021/[32]
FTO/CdS/Sb ₂ S ₃ /Spiro-OMeTAD/Au	Chemical bath deposition	/	8	2022/[16]
ITO/CdS/Sb ₂ S ₃ /PbS/C/Ag	Chemical bath deposition	/	0.13	2009/[33]
ITO/CdS/Sb ₂ S ₃ /Au	Thermal evaporation	O doping	4.8	2015/[34]
FTO/CdS/Sb ₂ S ₃ /Au	Rapid thermal evaporation	/	5.6	2015/[7]
ITO/CdS/Sb ₂ S ₃ /Au	Vapor transport deposition	/	7.6	2018/[35]
FTO/CdS/Sb ₂ S ₃ /Au	Rapid thermal evaporation	CuCl ₂ treatment	7.04	2018/[36]
Glass/Mo/Sb ₂ S ₃ /CdS/ITO	Magnetron sputtering	post-selenization	6.06	2019/[37]
Glass/Mo/Sb ₂ S ₃ /TiO ₂ /CdS/ZnO/AZO	Close spaced sublimation	/	9.2	2019/[38]
FTO/c-TiO ₂ /Sb ₂ S ₃ /Au	Close space sublimation	MgCl ₂ doping	7.3	2020/[39]
FTO/CdS/Sb ₂ S ₃ /Spiro-OMeTAD/Au	Thermal evaporation	Te doping	5.4	2020/[40]
FTO/CdS/Sb ₂ S ₃ /Spiro-OMeTAD/Au	Thermal evaporation	in situ selenization	6	2022/[41]
Glass/Mo/Sb ₂ S ₃ CdS/ZnO/AZO	Injection vapor deposition	/	10.12	2022/[42]
FTO/CdS/Sb ₂ S ₃ /Spiro-OMeTAD/Au	Chemical bath deposition	/	10.57	2022/[17]
FTO/c-TiO ₂ /mp-TiO ₂ /Sb ₂ (S,Se)3/PEDOT:PSST/Au	Chemical bath deposition	/	6.6	2014/[43]
FTO/CdS/Sb ₂ (S,Se)3/Spiro-OMeTAD/Au	Spin-coating	Water additive	7.42	2020/[27]
FTO/CdS/Sb ₂ (S,Se)3/Spiro-OMeTAD/Au	Sequential Co-evaporation deposition	/	8	2021/[16]
FTO/CdS/Sb ₂ (S,Se)3/Spiro-OMeTAD/Au	Hydrothermal deposition	/	10	2020/[8]
FTO/CdS/Zn(O,S)/Sb ₂ (S,Se)3/SpiroOMeTAD/Au	Hydrothermal deposition	/	10.7	2022/[11]

Not:c-TiO₂ and mp-TiO₂ stand for compact TiO₂ and mesoporous TiO₂

duce core–shell structured p–n junctions composed of Sb₂Se₃ nanorod arrays absorber along the [001] direction (Figure 4a and 4b),^[38] generating a certified efficiency of 9.2%.

Apart from the physical deposition, a novel hydrothermal deposition method was then developed to deposit high quality Sb₂X₃ films. Tang et al. firstly demonstrated this approach was able to obtain high quality Sb₂(S,Se)3 films with compact morphology, large grains, and favorable crystal orientation.^[8] Additionally, the ratio of S/Se can be easily modulated to regulate the bandgap of Sb₂(S,Se)3 films. Ultimately, a certified milestone PCE of 10.0% was achieved (Figure 4c and 4d), which was also listed as a world record in Detailed Balance (DB) Charts by Light Management in New Photovoltaic Materials (LMPV, Figure 5).^[44] Detailed inspection shows that the short-current density (J_{SC}) of Sb₂(S,Se)3 solar cell is closed to the Shockley–Queisser limit value (Figure 5b). However, open-circuit voltage (V_{OC}) and fill factor (FF) are much lower than the Shockley–Queisser limit values (Figure 5a and 5c). The origin of V_{OC} and FF loss is still unrevealed and is under investigation, for which have been summarized by some researchers.^[1, 14] Nevertheless, this achievement then drives the rapid development of Sb₂X₃ solar cells in recent years. Through modulating the nucleation process during hydrothermal process, more uniform Sb₂(S,Se)3 film with larger grain size as well as enhanced electrical properties was obtained and thus yielded a PCE of 10.5%.^[45] In spired by this result, Zhao et al. used post-treatment strategy to manipulate distribution of the S/Se in the films and created favorable energy alignment which facilitates the carrier transport, achieving a champion efficiency of 10.7%.^[11] On the basis of the hydrothermal method, Li et al. improved the CBD process to prepare Sb₂S₃ and Sb₂Se₃ films, yielding PCEs of 8% and 10.57%, respectively.^[16–17]

Those researches demonstrate that developing a novel de-

position method to prepare high-quality Sb₂X₃ is one of the most efficient approaches to elevate the PCE of Sb₂X₃ solar cells. During exploring deposition method, physical vapor deposition has always been the preferred method for depositing high-quality films because of the availability of dense and impurity-free films. It is known that physical vapor deposition process, such as thermal evaporation, magnetron sputtering, close spaced sublimation and so on, is an atomic deposition process, in which materials are evaporated from solid or liquid sources in the form of atoms or molecules, and transported to the substrate in the form of a vapor through vacuum or low-pressure gas environment. However, in the case of Sb₂X₃, owing to the difference in saturated vapor pressure of X and Sb₂X₃, Sb₂X₃ vapor may decompose to the vapor species composed of Sb₄, XSb, and X₂ during evaporation process.^[46] This process may result in ununiform distribution of elements and amount of deep energy level defects in the film, which requires effective posttreatment to remedy. As for the chemical deposition method, such as hydrothermal deposition, nucleation and crystal growth processes for depositing Sb₂X₃ film occur via ionic reaction in a sealed high-pressure environment using water as solvent medium, avoiding the drawbacks of physical vapor deposition. Therefore, at present, chemical deposition methods are considered as promising methods for fabricating high-efficient Sb₂X₃ solar cells.

Defect Characterization and Passivation

Apart from developing deposition method to prepare high-quality thin films, the deep level defect property in Sb₂X₃ is another issue should be pay more attentions. Basically, the deep level defect can trap the carriers, which is known as trap-assisted Shockley–Read–Hall (SRH) recombination, leading to shorten the photogenerated carrier lifetime. Addition-

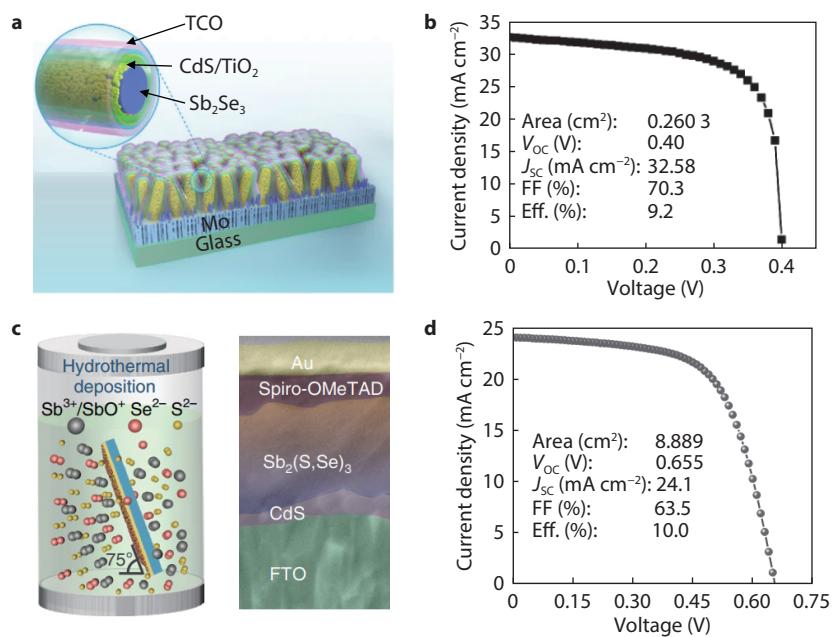


Fig. 4 **a** Schematic of the Sb_2Se_3 nanorod arrays on Mo-coated glass and $\text{Sb}_2\text{Se}_3/\text{CdS}$ core/shell nanorod array solar cells and **b** the corresponding J - V curve.^[38] Copyright 2019, Springer Nature. **c** Schematic of the hydrothermal deposition of $\text{Sb}_2(\text{S},\text{Se})_3$ in an autoclave along with the solar cell structure and **d** the corresponding J - V curve.^[8] Copyright 2020, Springer Nature.

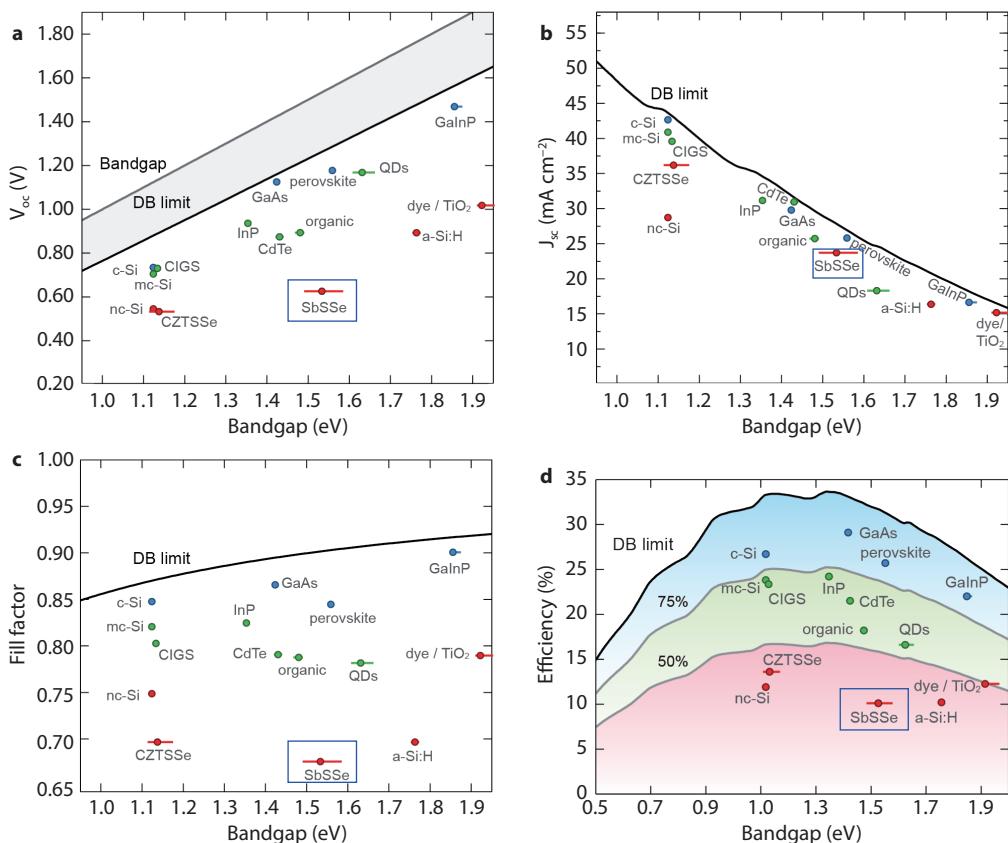


Fig. 5 Single-junction solar cell parameters are shown as a function of bandgap energy according to the Shockley-Queisser limit (solid lines) and experimental values for record efficiency cells: **a** Open-circuit voltage V_{OC} , **b** Short-circuit current J_{SC} , **c** Fill factor FF, and **d** power conversion efficiency PCE.^[44] Copyright 2022, LMPV.

ally, the Coulomb interaction between a carrier and a defect deflects the carrier, reducing the carriers' mobility.^[47] Therefore, the deep level defect is detrimental to the performance of solar cell device.^[32, 35] The Chen group pioneered investigated the defect properties in Sb_2X_3 via first-principle calculations and pointed out that the defect properties in Sb_2X_3 are complex and different from those in traditional photovoltaic semiconductors such as CdTe or GaAs (Figure 6a).^[48-49] Owing to the low symmetry crystal structure of Sb_2X_3 , the positions occupied by two Sb atoms and three X atoms are not equivalent to each other (Figure 6a). Therefore, the same type of point defects located on the nonequivalent atomic sites of Sb_2X_3 have different properties. Additionally, what troubles researchers most is that the defects such as Se vacancy, Se_{Sb} antisite and Sb_{Se} antisite are easily formed with deep levels and high concentrations, hence substantially restricting photovoltaic performance.

Based on theoretical research, defect passivation techniques along with defect characterization are implemented to investigate the defects properties associated with the performance of solar cell device from the experimental verification. Through the defect characterization technology, such as deep-level transient spectroscopy (DLTS) and temperature-dependent admittance spectral analysis, three kinds of deep defects (Sb_X , V_X , and Sb_i) with the concentration beyond 10^{14} cm^{-3} are generally observed in the cation-rich Sb_2X_3 film.^[32, 35, 41] Especially, Sb_X , V_X can cause serious recombination of carriers, which accounted for the large open-circuit voltage (V_{OC}) loss.^[50] In this regard, preparing anion-rich Sb_2X_3 film is thought as an efficient approach to passivate the defects. Therefore, in-situ anion supplementation,^[51-54] post-

treatment,^[55-57] and developing new methods for film preparation were utilized to passivate the defects in Sb_2X_3 films (Figure 6b).^[27] Additionally, element doping of Te and O is also applied to low the defect density (Figure 6c).^[34, 40] The typical passivation methods for defects are summarized in Table 1. Further theoretical calculation found that more Se vacancies can also be formed in Sb_2Se_3 under both Se-poor and Se-rich conditions.^[58] However, this result has not been verified by practical experimental studies. Through those variety of characterization and passivation strategies, the energy level location of each type of deep level defect in the bandgap can be basically determined. However, the understanding of control to defect type and property is not yet revealed. As a result, more attentions about the defect formation should be paid during films preparation to inhibit the generation of harmful anion vacancies.

Conclusions and Outlook

In summary, in the past few years, the research field of Sb_2X_3 solar cells saw a significant progress from the aspects of fundamental understanding, film fabrication, orientation control, defect characterization and passivation, and performance optimization. Based on that, the PCE of $Sb_2(S,Se)_3$ -based solar cells has broken the 10.0% bottleneck value. Although a great progress has been achieved on the PCE of Sb_2X_3 solar cells and its advantage in flexible device applications, the PCE of Sb_2X_3 solar cell still lags far from the state-of-the-art other thin-film solar cells like CdTe and CIGS solar cells. Therefore, enhancing the PCE is still the most urgent task at present for Sb_2X_3 solar cells. In this regard, based on our knowledge, we

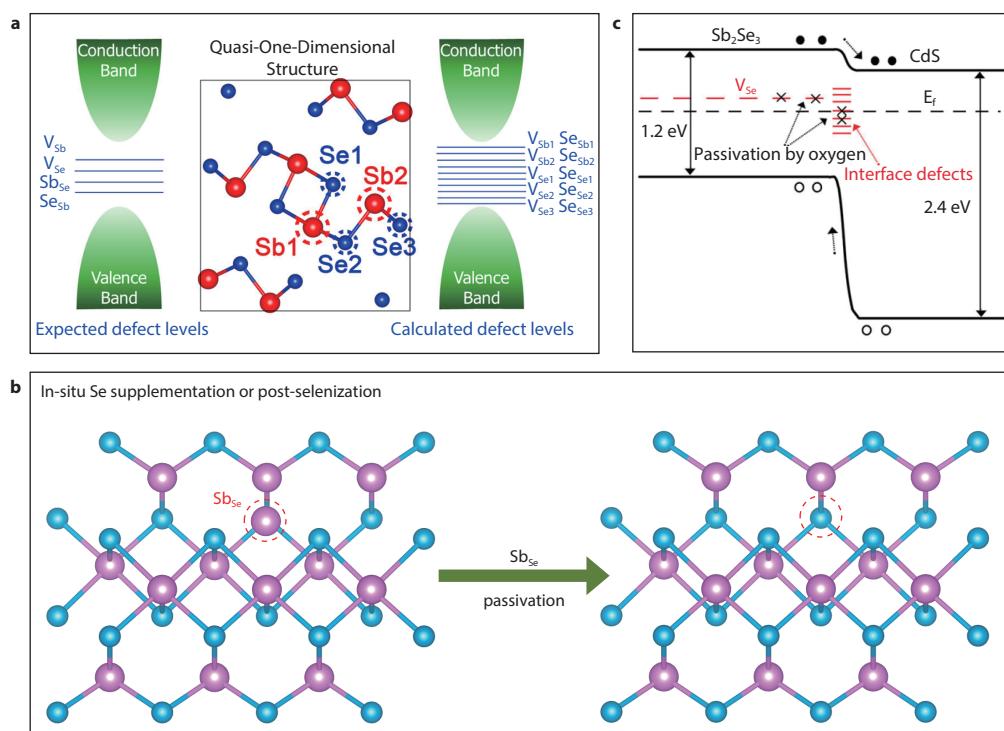


Fig. 6 **a** The types of defects derived from two nonequivalent Sb and three nonequivalent Se atomic sites in Sb_2Se_3 crystal.^[49] Copyright 2019, American Chemical Society. **b** Schematic of Sb_{Se} defect passivation through the method of *in situ* Se supplementation or post-selenization. **c** Sketchy band diagram between CdS and Sb_2Se_3 with and without doping oxygen.^[34] Copyright 2015, Wiley-VCH.

propose some suggestions for improving Sb_2X_3 based solar cells, which should be considered for the research in the future: (i) Novel synthesis approaches should be further explored to prepare high-quality Sb_2X_3 thin film with desirable orientations. It is expected that a new method could reduce the deep level defect density in the film. On the other hand, it can also improve the surface morphology as well as crystal orientation. (ii) Defect characterization and passivation should be further investigated. The better and deep understanding of defects could lead the researchers to overcome the limitation on PCE resulted from the defects. Although there are some researches on defects, these studies did not explain the formation mechanism of defect, nor can they accurately regulate defects. Therefore, combining the synthesis approach, defect passivation strategies, and theoretical calculation, the restraining effect of defects on PCE will be eliminated. (iv) The suitable electron and hole transport materials are other issues to be considered. Up to now, a fact is that the high-efficient Sb_2X_3 solar cells were exclusively based on CdS as electron transport material. As well known, the bandgap of CdS is 2.2 eV which restrict the short-wavelength quantum yield. Therefore, wide bandgap transport layer should be prioritized to permit the maximum light to reach the absorber. Additionally, Spiro-OMeTAD is widely used as hole transport material for high-efficient Sb_2X_3 solar cells. However, the intrinsic instability of organic Spiro-OMeTAD could cause serious device instability. In this regard, the alternative inorganic hole transport materials or hole transport material free devices should be tested on an urgent basis for better stability devices.

At the present stage, although the PCE of Sb_2X_3 cannot meet the requirement of commercial applications, we believe that the efficiency of the Sb_2X_3 solar cell will be further improved to meet the practical applications after further deep understanding the fundamental properties of Sb_2X_3 . In addition to the application of traditional photovoltaic power stations, the unique low dimensional crystal structure endows Sb_2X_3 with the intrinsic advantaged applications in flexible and portable device. It is anticipated that flexible Sb_2X_3 solar cells can be applied in various IoT scenarios include intelligent buildings, mobile health gadgets and BIPV.

ACKNOWLEDGMENT

This work was supported by the National Key Research and Development Program of China (Grant no. 2019YFA0405600), National Natural Science Foundation of China (Grant no. U19A2092, 22275180), Institute of Energy, Hefei Comprehensive National Science Center (Grant No. 21KZS212), Collaborative Innovation Program of Hefei Science Center, CAS, and Ningbo Natural Science Foundation (Grant No. 2021J205).

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

Dr. Lijian Zhang and Prof. Tao Chen proposed the layout. Dr. Lijian Zhang wrote the drafted manuscript. Prof. Tao Chen

supervised, revised, and edited the drafted manuscript. Dr. Chunyan Wu and Dr Wenhao Liang participated in the drawing of the charts and figures. All authors joined the discussion during the process of writing and revising the article. All authors read this manuscript and approve it for publication.

REFERENCES

1. C. Chen, J. Tang, *ACS Energy Lett.*, 2020, 5, 2294
2. M. A. Green, E. D. Dunlop, J. Hohl-Ebinger, M. Yoshita, N. Kopidakis, X. Hao, *Prog. Photovolt: Res. Appl.*, 2021, 29, 657
3. NREL, Best Research-Cell Efficiency Chart, <https://www.nrel.gov/pv/cell-efficiency.html>, July 2023.
4. L. Zhang, S. Cheng, J. Wang, T. Chen, *Sol. RRL*, 2022, 6, 2200561
5. X. Jin, Y. Fang, T. Salim, M. Feng, S. Hadke, S. W. Leow, T. C. Sum, L. H. Wong, *Adv. Funct. Mater.*, 2020, 30, 2002887
6. Y. C. Choi, D. U. Lee, J. H. Noh, E. K. Kim, S. I. Seok, *Adv. Funct. Mater.*, 2014, 24, 3587
7. Y. Zhou, L. Wang, S. Chen, S. Qin, X. Liu, J. Chen, D.-J. Xue, M. Luo, Y. Cao, Y. Cheng, E. H. Sargent, J. Tang, *Nat. Photonics*, 2015, 9, 409
8. R. Tang, X. Wang, W. Lian, J. Huang, Q. Wei, M. Huang, Y. Yin, C. Jiang, S. Yang, G. Xing, S. Chen, C. Zhu, X. Hao, M. A. Green, T. Chen, *Nat. Energy*, 2020, 5, 587
9. X. Wang, R. Tang, C. Wu, C. Zhu, T. Chen, *Journal of Energy Chemistry*, 2018, 27, 713
10. H. Dong, L. Zhang, B. Che, P. Xiao, H. Wang, C. Zhu, T. Chen, *ACS Appl. Opt. Mater.*, 2023, 1, 374
11. Y. Zhao, S. Wang, C. Jiang, C. Li, P. Xiao, R. Tang, J. Gong, G. Chen, T. Chen, J. Li, X. Xiao, *Adv. Energy Mater.*, 2022, 12, 2103015
12. A. Mavlonov, T. Razykov, F. Raziq, J. Gan, J. Chantana, Y. Kawano, T. Nishimura, H. Wei, A. Zakutayev, T. Minemoto, X. Zu, S. Li, L. Qiao, *Solar Energy*, 2020, 201, 227
13. U. A. Shah, S. Chen, G. M. G. Khalaf, Z. Jin, H. Song, *Adv. Funct. Mater.*, 2021, 31, 2100265
14. J. Dong, Y. Liu, Z. Wang, Y. Zhang, *Nano Select*, 2021, 2, 1818
15. C. Chen, K. Li, J. Tang, *Sol. RRL*, 2022, 6, 2200094
16. S. Wang, Y. Zhao, B. Che, C. Li, X. Chen, R. Tang, J. Gong, X. Wang, G. Chen, T. Chen, J. Li, X. Xiao, *Adv. Mater.*, 2022, 34, 2206242
17. Y. Zhao, S. Wang, C. Li, B. Che, X. Chen, H. Chen, R. Tang, X. Wang, G. Chen, T. Wang, J. Gong, T. Chen, X. Xiao, J. Li, *Energy Environ. Sci.*, 2022, 15, 5118
18. A. Polman, M. Knight, E. C. Garnett, B. Ehrler, W. C. Sinke, *Science*, 2016, 352, aad4424
19. L. Wang, D.-B. Li, K. Li, C. Chen, H.-X. Deng, L. Gao, Y. Zhao, F. Jiating, L. Li, F. Huang, Y. He, H. Song, G. Niu, J. Tang, *Nat. Energy*, 2017, 2, 17046
20. C. Chen, D. C. Bobela, Y. Yang, S. Lu, K. Zeng, C. Ge, B. Yang, L. Gao, Y. Zhao, M. C. Beard, J. Tang, *Frontiers of Optoelectronics*, 2017, 10, 18
21. X. Jin, Y. Fang, T. Salim, M. Feng, Z. Yuan, S. Hadke, T. C. Sum, L. H. Wong, *Adv. Mater.*, 2021, 33, 2104346
22. K. Li, F. Li, C. Chen, P. Jiang, S. Lu, S. Wang, Y. Lu, G. Tu, J. Guo, L. Shui, Z. Liu, B. Song, J. Tang, *Nano Energy*, 2021, 86, 106101
23. C. Chen, K. Li, F. Li, B. Wu, P. Jiang, H. Wu, S. Lu, G. Tu, Z. Liu, J. Tang, *ACS Photonics*, 2020, 7, 352
24. X. Wen, Z. Lu, L. Valdman, G. C. Wang, M. Washington, T. M. Lu, *ACS Appl Mater Interfaces*, 2020, 12, 35222
25. C. Wang, S. Lu, S. Li, S. Wang, X. Lin, J. Zhang, R. Kondrotas, K. Li, C. Chen, J. Tang, *Nano Energy*, 2020, 71, 104577
26. X. Wen, Z. Lu, G.-C. Wang, M. A. Washington, T.-M. Lu, *Nano En-*

ergy, 2021, 85, 106019

27. C. Wu, W. Lian, L. Zhang, H. Ding, C. Jiang, Y. Ma, W. Han, Y. Li, J. Zhu, T. Chen, C. Zhu, *Sol. RRL*, 2020, 4, 1900582
28. C. Wu, L. Zhang, H. Ding, H. Ju, X. Jin, X. Wang, C. Zhu, T. Chen, *Sol. Energy Mater. Sol. Cells*, 2018, 183, 52
29. D.-B. Li, X. Yin, C. R. Grice, L. Guan, Z. Song, C. Wang, C. Chen, K. Li, A. J. Cimaroli, R. A. Awani, D. Zhao, H. Song, W. Tang, Y. Yan, J. Tang, *Nano Energy*, 2018, 49, 346
30. Y. Itzhaik, O. Niitsoo, M. Page, G. Hodes, *J. Phys. Chem. C*, 2009, 113, 4254
31. M. Ishaq, H. Deng, U. Farooq, H. Zhang, X. Yang, U. A. Shah, H. Song, *Sol. RRL*, 2019, 3, 1900305
32. W. Lian, C. Jiang, Y. Yin, R. Tang, G. Li, L. Zhang, B. Che, T. Chen, *Nat. Commun.*, 2021, 12, 3260
33. S. Messina, M. Nair, P. Nair, *J. Electrochem. Soc.*, 2009, 156, H327
34. X. Liu, C. Chen, L. Wang, J. Zhong, M. Luo, J. Chen, D.-J. Xue, D. Li, Y. Zhou, J. Tang, *Prog. Photovolt: Res. Appl.*, 2015, 23, 1828
35. X. Wen, C. Chen, S. Lu, K. Li, R. Kondrotas, Y. Zhao, W. Chen, L. Gao, C. Wang, J. Zhang, G. Niu, J. Tang, *Nat. Commun.*, 2018, 9, 2179
36. C. Chen, K. Li, S. Chen, L. Wang, S. Lu, Y. Liu, D. Li, H. Song, J. Tang, *ACS Energy Lett.*, 2018, 3, 2335
37. R. Tang, Z.-H. Zheng, Z.-H. Su, X.-J. Li, Y.-D. Wei, X.-H. Zhang, Y.-Q. Fu, J.-T. Luo, P. Fan, G.-X. Liang, *Nano Energy*, 2019, 64, 103929
38. Z. Li, X. Liang, G. Li, H. Liu, H. Zhang, J. Guo, J. Chen, K. Shen, X. San, W. Yu, R. E. I. Schropp, Y. Mai, *Nat. Commun.*, 2019, 10, 125
39. T. D. C. Hobson, L. J. Phillips, O. S. Hutter, H. Shiel, J. E. N. Swallow, C. N. Savory, P. K. Nayak, S. Mariotti, B. Das, L. Bowen, L. A. H. Jones, T. J. Featherstone, M. J. Smiles, M. A. Farnworth, G. Zoppi, P. K. Thakur, T.-L. Lee, H. J. Snaith, C. Leighton, D. O. Scanlon, V. R. Dhanak, K. Durose, T. D. Veal, J. D. Major, *Chem. Mater.*, 2020, 32, 2621
40. Y. Ma, B. Tang, W. Lian, C. Wu, X. Wang, H. Ju, C. Zhu, F. Fan, T. Chen, *J. Mater. Chem. A*, 2020, 8, 6510
41. W. Lian, R. Cao, G. Li, H. Cai, Z. Cai, R. Tang, C. Zhu, S. Yang, T. Chen, *Adv. Sci.*, 2022, 9, 2105268
42. Z. Duan, X. Liang, Y. Feng, H. Ma, B. Liang, Y. Wang, S. Luo, S. Wang, R. E. I. Schropp, Y. Mai, Z. Li, *Adv. Mater.*, 2022, 34, e2202969
43. Y. C. Choi, Y. H. Lee, S. H. Im, J. H. Noh, T. N. Mandal, W. S. Yang, S. I. Seok, *Adv. Energy Mater.*, 2014, 4, 1301680
44. LMPV, Detailed Balance (DB) Charts, <https://www.lmpv.nl/db/>, July 2023.
45. X. Wang, R. Tang, C. Jiang, W. Lian, H. Ju, G. Jiang, Z. Li, C. Zhu, T. Chen, *Adv. Energy Mater.*, 2020, 10, 2002341
46. X. Liu, J. Chen, M. Luo, M. Leng, Z. Xia, Y. Zhou, S. Qin, D. J. Xue, L. Lv, H. Huang, D. Niu, J. Tang, *ACS Appl. Mater. Interfaces*, 2014, 6, 10687
47. J. M. Ball, A. Petrozza, *Nat. Energy*, 2016, 1, 16149
48. Z. Cai, C.-M. Dai, S. Chen, *Sol. RRL*, 2020, 4, 1900503
49. M. Huang, P. Xu, D. Han, J. Tang, S. Chen, *ACS Appl. Mater. Interfaces*, 2019, 11, 15564
50. C. Chen, L. Wang, L. Gao, D. Nam, D. Li, K. Li, Y. Zhao, C. Ge, H. Cheong, H. Liu, H. Song, J. Tang, *ACS Energy Lett.*, 2017, 2, 2125
51. M. Leng, M. Luo, C. Chen, S. Qin, J. Chen, J. Zhong, J. Tang, *Appl. Phys. Lett.*, 2014, 105, 083905
52. A. Shongalova, M. R. Correia, J. P. Teixeira, J. P. Leitão, J. C. González, S. Ranjbar, S. Garud, B. Vermang, J. M. V. Cunha, P. M. P. Salomé, P. A. Fernandes, *Sol. Energy Mater. Sol. Cells*, 2018, 187, 219
53. A. Maiti, S. Chatterjee, A. J. Pal, *ACS Appl. Energ. Mater.*, 2020, 3, 810
54. J. Kim, S. Ji, Y. Jang, G. Jeong, J. Choi, D. Kim, S.-W. Nam, B. Shin, *Sol. RRL*, 2021, 5, 2100327
55. S. Yuan, H. Deng, X. Yang, C. Hu, J. Khan, W. Ye, J. Tang, H. Song, *ACS Photonics*, 2017, 4, 2862
56. H. Deng, S. Yuan, X. Yang, F. Cai, C. Hu, K. Qiao, J. Zhang, J. Tang, H. Song, Z. He, *Materials Today Energy*, 2017, 3, 15
57. G.-X. Liang, Y.-D. Luo, S. Chen, R. Tang, Z.-H. Zheng, X.-J. Li, X.-S. Liu, Y.-K. Liu, Y.-F. Li, X.-Y. Chen, Z.-H. Su, X.-H. Zhang, H.-L. Ma, P. Fan, *Nano Energy*, 2020, 73, 104806
58. M. Huang, Z. Cai, S. Wang, X. G. Gong, S. H. Wei, S. Chen, *Small*, 2021, 17, 2102429



©2024 The Authors. Energy Lab is published by Lab Academic Press. This is an open access article under the terms of the Creative Commons Attribution License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

Biographies



Lijian Zhang obtained his PhD degree from University of Science and Technology of China in 2019. His work focuses on metal chalcogenides solar cells.



Tao Chen obtained his PhD degree from Nanyang Technological University, Singapore in 2010. In 2011, he joined Department of Physics, Chinese University of Hong Kong as a research assistant professor. Since 2015, he has been working in Department of Materials Science and Engineering, University of Science and Technology of China as a full professor. His work focuses on metal chalcogenides solar cells.