

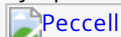
Symposium (Oral) | Symposium : New direction of perovskite solar cells

📅 Mon. Sep 16, 2024 1:30 PM - 6:30 PM JST | Mon. Sep 16, 2024 4:30 AM - 9:30 AM UTC 🏠 C41 (Hotel Nikko 4F)

[16p-C41-1~12] New direction of perovskite solar cells

Tetsuhiko Miyadera(AIST), Hiroko Takeoka(Sophia Univ.), Yasuhiro Shirai(NIMS), Shuxia Tao(Eindhoven University of Technology)

Symposium Sponsor



◆ English Presentation

1:30 PM - 2:00 PM JST | 4:30 AM - 5:00 AM UTC

[16p-C41-1]

Materials theory of halide perovskites: defect and chirality

○Shuxia Tao¹ (1.Materials Simulation & Modelling, Department of Applied Physics, Eindhoven University of Technology, The Netherlands)

◆ English Presentation

2:00 PM - 2:30 PM JST | 5:00 AM - 5:30 AM UTC

[16p-C41-2]

Crystal growth in perovskite solar cells

○Tetsuhiko Miyadera¹ (1.AIST)

◆ English Presentation

2:30 PM - 3:00 PM JST | 5:30 AM - 6:00 AM UTC

[16p-C41-3]

Molecular engineering of interfaces for efficient and stable perovskite solar cells

○Somin Park¹ (1.National Univ. of Singapore)

◆ English Presentation

3:15 PM - 3:45 PM JST | 6:15 AM - 6:45 AM UTC

[16p-C41-4]

Structural Control of Pb or Sn-based 2D Perovskite Compounds

○Yuko Takeoka¹, Daizo Hishida¹, Hirona Kobayashi¹, Chunqing Li¹, Masahiro Fujita¹, Masahiro Rikukawa¹ (1.Sophia University)

◆ English Presentation

3:45 PM - 4:15 PM JST | 6:45 AM - 7:15 AM UTC

[16p-C41-5]

Two-Dimensional (2D) Tin Halide Perovskite Semiconductors for Lasing

○Enzheng Shi¹ (1.Westlake University)

◆ English Presentation

4:30 PM - 4:45 PM JST | 7:30 AM - 7:45 AM UTC

[16p-C41-6]

Understanding the stability of perovskite solar cells through an adlayer of FAPbI₃ quantum dots.

○Svrcek Vladimir¹, Bruno Alessi¹, Zhihao Xu¹, Calum McDonald¹, Takuya Matsui¹ (1.AIST Tsukuba)

◆ English Presentation

4:45 PM - 5:00 PM JST | 7:45 AM - 8:00 AM UTC

[16p-C41-7]

Rapid PbI₂ Precursor Evaporation toward Industrial Perovskite Solar Cells

○(P)Abduheber Mirzehmet¹, Calum McDonald¹, Vladimir Svrcek¹, Hitoshi Sai¹, Takurou Murakami¹, Takuya Matsui¹ (1.AIST)

◆ English Presentation

5:00 PM - 5:15 PM JST | 8:00 AM - 8:15 AM UTC

[16p-C41-8]

PbS-CQD Incorporated Perovskite (MASnI₃) Solar Cell with s-SWCNT as HTL

○(M2)Md. Faiaad Rahman¹, Ahmed Zubair¹ (1.Bangladesh University of Engineering and Technology)

◆ English Presentation

5:15 PM - 5:30 PM JST | 8:15 AM - 8:30 AM UTC

[16p-C41-9]

Organic and Perovskite Solar Cells Utilizing Carbon Nanotubes Thin-film Electrode

○Yutaka Matsuo^{1,2} (1.Nagoya Univ., 2.i-MI, Nagoya Univ.)

◆ English Presentation

5:45 PM - 6:00 PM JST | 8:45 AM - 9:00 AM UTC

[16p-C41-10]

Electronic and Optical Properties and Defect Investigation of MASnX₃ (X = Cl, Br, and I) Perovskite Structures as Solar Cell Absorber

○Qing Wang¹, Aimi Hiratsuka², Satoshi Iikubo¹ (1.Kyushu Univ., 2.Kyushu Inst. of Tech)

◆ English Presentation

6:00 PM - 6:15 PM JST | 9:00 AM - 9:15 AM UTC

[16p-C41-11]

Performance Optimization of Ge: Sn (1:1) Perovskite Solar Cells Using Doping Engineering

○(PC)Ajay Kumar Baranwal¹, Qing Shen¹, Shuzi Hayase¹ (1.Electro-Comm. Univ.)

◆ English Presentation

6:15 PM - 6:30 PM JST | 9:15 AM - 9:30 AM UTC

[16p-C41-12]

Resolving the Light and the Thermal Stability Issues in the Tin-Lead Perovskite Solar Cells by Manipulating the Carrier Selective Layers with Dopant and/or Passivation

○(PC)Shahrir Razey Sahamir¹, Takeru Bessho², Hiroshi Segawa², Qing Shen¹, Shuzi Hayase¹ (1.Univ. of Electro-Com, 2.Univ. of Tokyo)

Materials Theory of Halide Perovskites: Defect and Chirality

Associate Professor Shuxia Tao, Materials Simulation & Modelling, Department of Applied Physics, Eindhoven University of Technology, The Netherlands

Abstract

Halide perovskites have gained prominence in optoelectronics and quantum materials due to their chemical versatility, which allows for a broad range of interactions with light, electrons, spins, and lattice vibrations. My team employs first-principles methods like density functional theory, tight-binding models, and machine learning-accelerated molecular dynamics to explore their complex structure-property relationships. We focus on defect chemistry to enhance PV solar cell efficiency and stability, identifying and mitigating defects that cause losses and degradation through compositional adjustments and surface treatments.

Additionally, we explore the chirality of perovskites, using chiral ligands to introduce properties like chiral-induced spin selectivity and enhancing chiral optical activity. This exploration aims to harness these distinctive properties for pioneering applications in spin LEDs and chiral photodetectors, driven by a deep understanding of the relation between structural features and optoelectronic properties.

ペロブスカイト太陽電池と結晶成長

Crystal growth in perovskite solar cells

産総研 ○宮寺 哲彦

AIST, °Tetsuhiko Miyadera

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Perovskite solar cells have been developing very rapidly and are already in the phase of mass production. Although its power conversion efficiency has been rapidly increasing, more fundamental research is needed for further development in order to distribute reliable products to the market. Especially, fabrication control of perovskite crystal is important because the reproducibility of the device performance is important issue for the perovskite solar cells. We have been focusing on vacuum deposition, aiming for precise control of perovskite fabrication. We also conducted real-time X-ray diffraction analysis using the synchrotron facility SPring-8 to investigate the dynamics of the perovskite crystallization process from the viewpoint of both solution process ^[1] and vacuum deposition process ^[2].

We implemented IR-laser deposition for the deposition of perovskite and demonstrated the benefit of the use of laser instead of resistive heater for the controllability of deposition rate of methylammonium iodide ^[3]. We also demonstrated the epitaxial growth of perovskite, where $\text{CH}_3\text{NH}_3\text{PbI}_3$ crystals with atomically flat morphology were achieved ^[4]. Layer-by-layer growth during laser-deposition process is investigated by real-time XRD analysis ^[2]. We are attempting to fabricate the solar cells using this crystallization method ^[5].

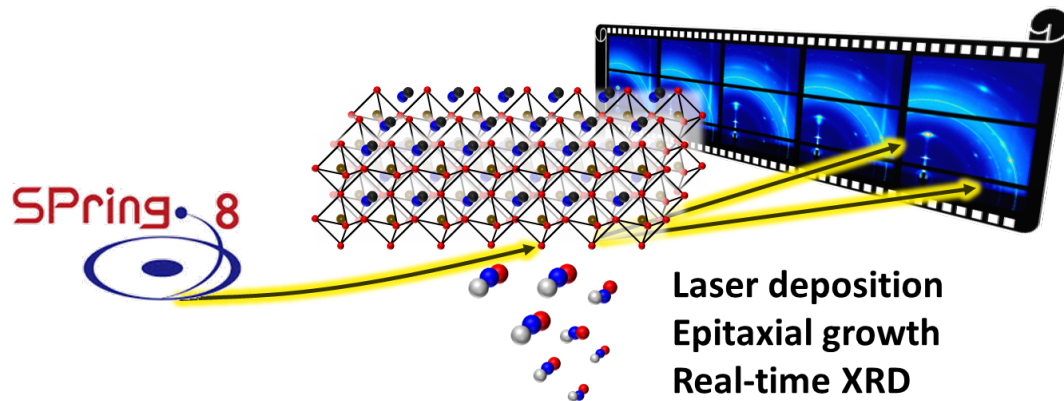


Fig: Schematic illustration of our research concept.

References:

- [1] T. Miyadera et al., *Nano Lett.* 15, (2015) 5630-5634.
- [2] T. Miyadera, et al., *ACS Appl. Mater. Int.* 13 (2021) 22559–22566.
- [3] T. Miyadera, et al., *ACS Appl. Mater. Int.* 8 (2016) 26013-26018.
- [4] T. Miyadera, et al., *APL Mater.* 8 (2020) 041104.
- [5] I. Kamikawa et al., *Jpn. J. Appl. Phys.* 63 (2024) 03SP86.

Extended Abstract of the Japan Society of Applied Physics**Molecular engineering of interfaces for efficient and stable perovskite solar cells****Somin Park****Department of Chemistry, National University of Singapore****Email: Somin.park.819@gmail.com**

Symposium Name: T14 New direction of perovskite solar cells

Abstract: Interfacial two- and three-dimensional heterostructures that incorporate ammonium ligand intercalation have enabled rapid progress toward the goal of uniting performance with stability in perovskite solar cells. However, as the field continues to seek ever-higher durability, additional tools that avoid progressive ligand intercalation are needed to minimize degradation at high temperatures. In this talk, I will present how the molecular structure, varying both the tail groups and alkyl chain lengths, influences the surface interactions and its energetics. I will focus on developing a series of anilinium derivatives that exhibit minimal reactivity with perovskites, leading to improved stability at the interface. Additionally, I will present our physical insights into the co-adsorbent self-assembled monolayers that reduce interfacial recombination and enhance electronic structures.

Structural Control of Pb or Sn-based 2D Perovskite Compounds

Sophia Univ., ^oYuko Takeoka¹, Daizo Hishida¹, Hirona Kobayashi¹, Li Chunqing,

Masahiro Yoshizawa-Fujita, Masahiro Rikukawa

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Organic-inorganic perovskite compounds have attracted much attention since their initial application in photovoltaic solar cells by Miyasaka et. al. Among the Pb-based perovskites, three-dimensional (3D) organic-inorganic perovskites have been mainly used for solar cells. However, they are easily affected by moisture, oxygen, and heat, and are susceptible to degradation by water. To address this issue, utilization of lower-dimensional structures is expected. Our group have reported the series of organic-inorganic perovskites having three-, two-, one-, and zero-dimensional (3D, 2D, 1D, and 0D) network of lead halide octahedra $[\text{PbX}_6]^{4-}$ using various kinds of organic amines.^{1,2} Up to now, we can find out that the 2D and quasi-2D perovskite structures show high stability against moisture, which enables no degradation of exciton absorption peak and layered structure after one year as shown in Figure 1.

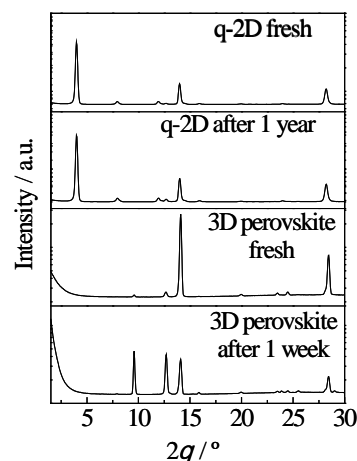


Figure 1. X-ray diffraction patterns of q-2D and 3D perovskite films as prepared and after storing.

On the other hand, orientation control is very important to use 2D and q-2D compounds as light absorbers for photovoltaic solar cells. Because 2D perovskites possess an organic amine layer that acts as an insulator and the $[\text{PbX}_6]^{4-}$ layers are connected two-dimensionally, the diffusion of photo generated carriers is limited to two directions. Typically, 2D and q-2D perovskites have a strong tendency to orient parallel to the substrate, rendering the migration of transport carriers in the vertical direction difficult.

To overcome this problem, based on the idea that the orientation of 2D and q-2D perovskites is affected by the crystallization process and the balance of various interactions such as ionic bonding, hydrogen bonding and van der Waals interactions, we prepared 2D and q-2D perovskites by using various organic ammoniums and several coting methods.^{3, 4} In some systems, the orientation of inorganic sheets was changed from parallel. In addition, we focused on the effect of symmetricity and ammonium grade (primary, secondary) on the orientation. In this presentation, the detailed analysis of these systems will be discussed.

References

- 1) Y. Takeoka, K. Asai, M. Rikukawa, and K. Sanui: *Bull. Chem. Soc. Jpn.* **79**, 10, (2006) 1607.
- 2) Y. Takeoka, K. Asai, M. Rikukawa, and K. Sanui, *Chem. Lett.*, 34, 4 (2005) 602.
- 3) R. Hamaguchi, M. Yoshizawa-Fujita, T. Miyasaka, H. Kunugita, K. Ema, Y. Takeoka and M. Rikukawa, *Chem. Commun.*, **53**, (2017) 4366.
- 4) M. Akiyoshi, M. Yoshizawa-Fujita, Y. Takeoka, and M. Rikukawa: *Chem. Comm.* **57** (2021) 3395.

Acknowledgements

This work was partly supported by JST-ALCA-Next Program Grant Number JPMJAN23B2, Japan.

Two-Dimensional (2D) Tin Halide Perovskite Semiconductors for Lasing

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Due to the highly tunable band structure, excellent optoelectronic properties, and low toxicity, tin halide perovskite semiconductors have attracted tremendous attention in the field of optoelectronics. In this talk, by employing the slow-cooling crystallization method and tuning the polarity of the growth solution, we obtained phase-pure 2D tin halide perovskite single crystals with tunable quantum-well thickness (n value) and hydrophobic π -conjugated organic ligands. Based on these lead-free perovskites, photogenerated carrier behaviors and lasing performance are systematically studied. Both high- n value ($n > 1$) and $n = 1$ tin perovskite thin flakes were successfully optically pumped to lase. Furthermore, the lasing from 2D tin perovskites could be maintained up to room temperature. Our findings highlight the tremendous potential of 2D tin perovskites as promising candidates for high-performance lasers.

Understanding the stability of perovskite solar cells through an adlayer of FAPbI₃ quantum dots.

Vladimir Svrcek¹, Bruno Alessi¹, Zhihao Xu¹, Calum McDonald¹, and Takuya Matsui¹

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To enhance the stability of Formamidinium lead iodide (FAPbI₃) hybrid solar cells without compromising efficiency, we propose introducing a thin adlayer of FAPbI₃ quantum dots (QDs) (< 100 nm) on bulk FAPbI₃ film solar cells. In this study, we assess the specific impact of ligands and fs laser-engineered FAPbI₃ QDs adlayer on stability and performance. By carefully controlling particle size and transport properties through the synthesis and ligand engineering, we can effectively increase the energy gap of FAPbI₃-QDs. We report that substituting Octadecene with Octene as the supporting solvent at the same injection temperature leads to effective ligand exchange. Using Octene resulted in superior optical and transport properties. When applied to solar cells, FAPbI₃ QDs with Octene exhibited superior properties in all parameters (PCE, J_{sc}, Voc) except for the fill factor (FF) compared to those with Octadecene. This drawback was overcome by femtosecond (fs) pulsed laser treatment of the FAPbI₃ QDs.

Another crucial aspect is enhancing the stability of the FAPbI₃ perovskite layer with the fs laser-treated FAPbI₃-QDs adlayer. Unlike films containing a QDs adlayer, all solar cell parameters for the FAPbI₃ film were depressed even after storage in the dark in a dry box (RH~ 1%) only. This degradation further increased when the solar cells were placed in a humid chamber. Figure 1a shows the power conversion efficiency characteristics of solar cells exposed to continuous light for 0, 24, and 110 hours in a humid chamber (RH 30 %T=28°C). Our findings indicate a significant improvement in stability when utilizing the QDs adlayer compared to standard FAPbI₃ perovskite material, more pronounced for fs treated FAPbI₃ QDs. It also implies that air stable FAPbI₃ QDs not only broaden the energy gap but also act as a passivation layer for the FAPbI₃ layer surface, enhancing compatibility with the hole transport layer. Furthermore, Figures 1b and 1c show XRD spectra and peak identification for three sample types as a function of 24h exposure in a humid chamber. The QDs adlayer slows down the alpha to delta transition when films are exposed to light soaking in a humid chamber. Additionally, FAPbI₃ QDs treated with fs laser slow down the formation of PbI₂.

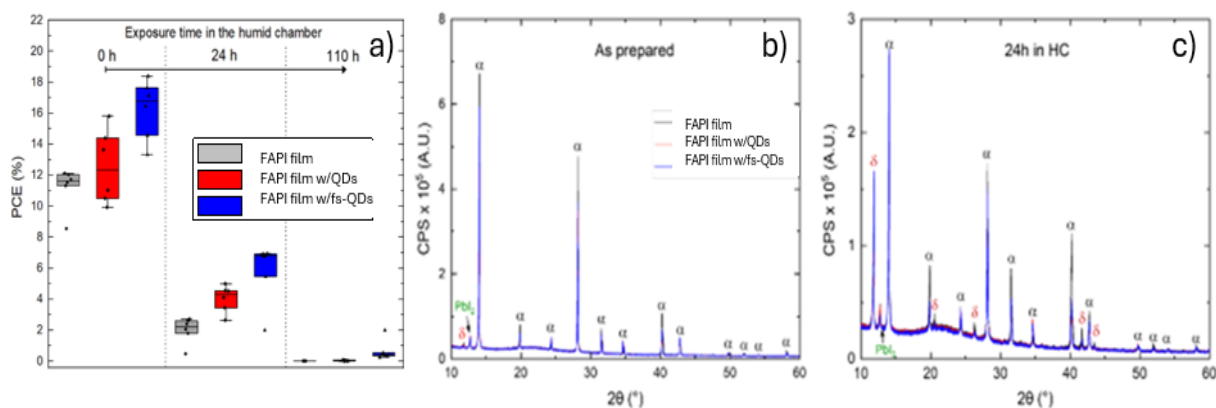


Figure 1. (a) Power conversion efficiency (PCE) of solar cells containing FAPbI₃, FAPbI₃ with an as-prepared QDs adlayer, and FAPbI₃ with an fs laser-treated FAPbI₃ QDs adlayer. (b) XRD spectra and peak identification for the three types of samples as prepared, and (c) after 24 hours of exposure to a humid chamber.

Rapid PbI₂ Precursor Evaporation toward Industrial Perovskite Solar Cells

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Accelerating the adoption of perovskite solar cells is crucial for the evolution of renewable energy technologies. Achieving high-performance perovskite solar cells necessitates scalable processing of the perovskite light absorber, compatible with existing deposition techniques. Fast deposition offers advantages such as reduced production time, increased throughput, and lower manufacturing costs in industrial applications. Methods for forming perovskite thin films include solution processing (bar coating, spray, inkjet, etc.), thermal evaporation, and hybrid processes. A common hybrid process involves evaporating metal halide precursors like PbI₂ and then coating them with an organic halide solution (FAMAIBrCl in isopropanol) to form perovskite crystals [1,2]. This method has recently attracted attention for its ability to enhance film coverage on substrates and produce uniform perovskite films over large areas, potentially enabling the production of fully textured tandem perovskite/Si solar cells.

In this study, we used a hybrid evaporation-solution process to fabricate perovskite thin films. We first evaporated ~300-nm-thick PbI₂ films at various rates, with the shortest duration for the highest rate being about 8 minutes. (Fig.1) For the solution process, we tentatively applied a spin-coating method to coat the PbI₂ film with an organic halide solution (FAMAIBrCl in isopropanol). We found that increasing the evaporation rate resulted in an improvement in overall power conversion efficiency (PCE), comparable to that of spin-coated perovskite. The results indicate that even higher evaporation rates are possible while maintaining the solar cell performance, which is beneficial for industrial applications.

[1] Fu, F., *et al. Nat Commun.* **6**, 8932 (2015).

[2] Fu, F., *et al. Nat. Energy* **2**, 16190 (2017).

Acknowledgment: This work was conducted under a project commissioned by NEDO, Japan.

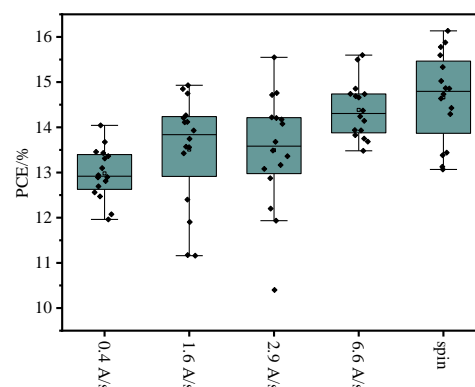


Fig. 1. Box charts illustrating the statistical distribution of power conversion efficiency (PCE) as a function the average evaporation rate of PbI₂ layers.

PbS-CQD Incorporated Perovskite (MASnI₃) Solar Cell with s-SWCNT as HTL

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Abstract— In the pursuit of advancing solar cell technology, a novel p-i-n perovskite solar cell design is proposed featuring methyl ammonium tin iodide (MASnI₃) as the primary light-absorbing layer, PbS CQDs as the secondary absorber, (6,5)-SWCNT as HTL. For an optimized thickness 100 nm for MASnI₃, a maximum PCE of 22.203%, with J_{sc} of 30.31 mA/cm², V_{oc} of 0.862 V.

I. Introduction

The main focus of this design is the inclusion of MASnI₃, a perovskite material, as the primary absorber with a bandgap of 1.3 eV and an electron affinity (χ_p) of 3.93 eV [1], along with PbS colloidal quantum dots (CQDs) that serve as a secondary layer for absorbing light with band gap of 1.3 eV [2,3]. The incorporation of (6,5) SWCNT with 1.3 eV bandgap and electron affinity of 3.8 eV as the hole transport layer (HTL) to create a blocking barrier for electron diffusion [4] is a notable innovation that attempts to enhance the performance of the cell.

II. Materials and Methods

For modelling and building the structure, TiO₂ was used as the electron transport layer (ETL), MASnI₃ as the primary absorber, (6,5) SWCNT, a semiconducting SWCNT (s-SWCNT), as the HTL, colloidal PbS quantum dots as the secondary absorber, ITO as the front contact, and graphite as back contact as shown in Fig 1(a). Optoelectronic simulations were conducted in 3D at constant temperature (300K) using Ansys Lumerical tools. The optical simulation was performed, using FDTD methods to solve Maxwell's wave equations with Dirichlet and Neumann boundary conditions. Periodic conditions are applied in X and Y directions and a phase matched layer (PML) in the Z direction, under AM1.5G solar spectrum illumination (300 – 1000 nm). For electrical simulation, performance parameters like power conversion efficiency (PCE), short circuit current density (J_{sc}), open circuit voltage (V_{oc}), and fill factor (FF) were calculated using Poisson's equation, drift-diffusion equations, and continuity equations.

III. Results and Discussion

For the initial opto-electronic simulation, layer thicknesses of ITO/TiO₂/MASnI₃/PbS-CQDs/s-SWCNT/C were set as 50nm, 90 nm, 200 nm, 800 nm, 800 nm, and 100 nm respectively. After executing simulations keeping centre-to-centre distance (CCD) between nanotubes at 20 nm, the device achieved a PCE of 17.48% with J_{sc} of 30.50 mA/cm², V_{oc} of 0.877 V, and FF of 65.36%. Fig. 1 (b) illustrate optical carrier generation rate, and (c) spectral power absorption with respect to the AM1.5G solar spectrum. Device performance results showed that increasing CCD, decreased performance of cell as the (6,5) SWCNT became less dense, reducing hole collection. Afterward, the thickness of the MASnI₃ layer was varied from 50 nm to 700 nm with $N_A = 1 \times 10^{16}$ cm⁻³ as shown in Fig. 1(d), keeping PbS-CQDs and (6,5) SWCNT thickness constant. The optimal MASnI₃ thickness was 100 nm, yielding a PCE of 22.18% with J_{sc} of 30.309 mA/cm², V_{oc} of 0.862V, and FF of 84.91%. The PCE peaked at 100 nm and declined beyond this due to increased electron-hole recombination and reduced hole collection. For J_{sc} , it increased with MASnI₃ thickness up to 350 nm before decreasing. The diffusion lengths (L_n and L_p) for MASnI₃ were calculated to be 322 nm, suggesting optimal electron and hole travel distances, and a maximum J_{sc} of 32.78 mA/cm². V_{oc} decreased slightly with MASnI₃

thickness up to 250 nm, then increased up to 700 nm, correlating with J_{sc} changes.

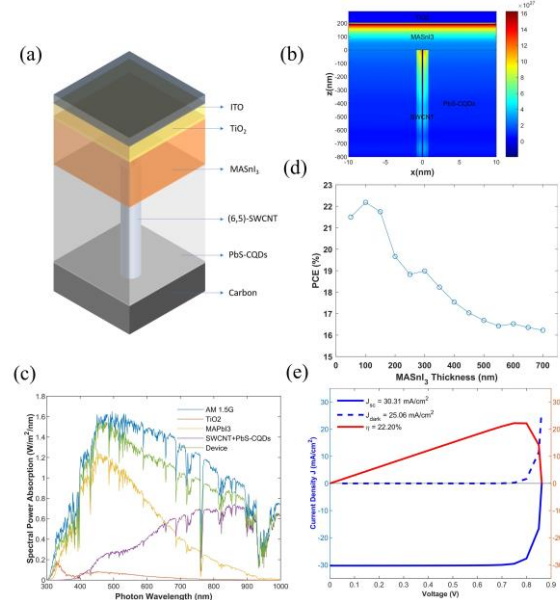


Fig. 1: (a) Device architecture. (b) Carrier generation rate, G (m⁻³s⁻¹) in X-Z cross-section (c) Spectral power absorption density, P_{abs} vs photon wavelength for different absorber layer for AM1.5G solar spectrum. (d) PCE vs thickness of MASnI₃. (e) J-V and PCE(η)-V curves.

FF consistently decreased with increased thickness. To explore the effect of acceptor doping density (N_A) of MASnI₃ on device performance, N_A was varied from 5×10^{13} cm⁻³ to 5×10^{16} cm⁻³. Performance remained stable up to 5×10^{15} cm⁻³, slightly decreasing marginally after 1×10^{16} cm⁻³. The optimal output was extracted with a PCE of 22.203%, J_{sc} of 30.31 mA/cm², V_{oc} of 0.862V, and FF of 84.98% with calculated dark current density (J_{dark}) of 25.06 mA/cm².

IV. Conclusions

In this work, the impact of incorporation of PbS-CQD, density of carbon nanotubes as HTL in perovskite solar, and thickness and effective doping density of MASnI₃ on the performance of device characteristics has been investigated. Further research can be implemented to optimize the device's efficacy even more.

References

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- [3] Majdi, M., Eskandari, M., & Fathi, D. (2021). Textured HTM-free perovskite/PbS quantum dot solar cell: Optical and electrical efficiency improvement by light trapping control. *Solar Energy*, 230, 618-627.
- [4] Lee, E. J., Lee, W., Yun, T. H., You, H. R., Kim, H. J., Yu, H. N., ... & Choi, J. (2024). Suppression of Thermally Induced Surface Traps in Colloidal Quantum Dot Solids via Ultrafast Pulsed Light. *Small*, 2400380.

単層カーボンナノチューブ薄膜透明電極を用いた有機薄膜およびペロ
ブスカイト太陽電池

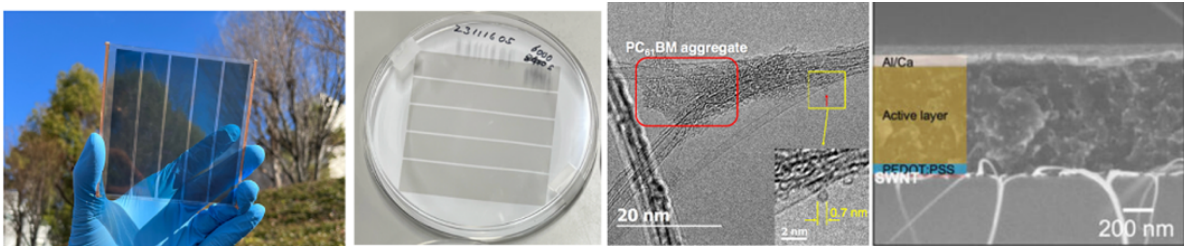
Organic and Perovskite Solar Cells Utilizing Carbon Nanotubes Thin-film Electrode

名大院工¹, 名大マテイノベ研² °松尾 豊^{1,2}

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単層カーボンナノチューブ (CNT) 薄膜透明電極を用いた有機薄膜太陽電池 (OPV) およびペ
ロブスカイト太陽電池 (PSC) の研究に関する最近の取り組みについて紹介する。特に CNT 薄膜
透明電極を、電子を受け取る側の電極 (カソード) として用いるための CNT に対する n ドープに
ついて詳細に議論する。



カーボンナノチューブ薄膜透明電極OPV n型CNT電極 ITOフリー下部CNT電極

図1. 両面受光型 10cm 角 CNT-OPV セミモジュール, CNT カソード, ITO を用いない OPV

表1. OPV or PSC, 順型 or 逆型, 上部 or 下部電極の計 8 種類の CNT-OPV, CNT-PSC

種類	下部電極 (透明電極)	上部電極 (裏面電極)	発電層材料	電子 輸送層	正孔 輸送層	変換 効率
順型OPV	ITO p型CNT	n型CNT Al	— PV-D4610/PCBM	— LiF	— PEDOT:PSS	— 8.0%
逆型OPV	ITO n型CNT	p型CNT Ag	PV-D4610/PCBM PV-D4610 /PCBM	ZnO ZnO	PEDOT:PSS PEDOT:PSS	5.5% 2.9%
順型PSC	ITO n型CNT	p型CNT Ag	MAPbI ₃ —	C ₆₀ —	(spiro) —	17.0% —
逆型PSC	ITO p型CNT	n型CNT Cu	MAPbI ₃ MAPbI ₃	PCBM C ₆₀	PEDOT:PSS PTAA	8.0% 17.2%
<両面CNT太陽電池>						
逆型PSC	p型CNT	n型CNT	MAPbI ₃	(PCBM)	(P3HT) PEDOT:PSS	7.3%

参考文献

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2) 大岩詩門, 松尾 豊, 車載テクノロジー 2023, Vol.10, No.11 (2023 年 8 月号), P58-61.

MASnX₃ (X=Cl, Br, I) ペロブスカイト構造の太陽電池光吸収層としての電子・光学的性質と欠陥評価

Electronic and Optical Properties and Defect Investigation of MASnX₃ (X = Cl, Br, and I) Perovskite Structures as Solar Cell Absorber

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Organic-inorganic hybrid perovskite materials, such as MAPbI₃, have demonstrated exceptional potential as photovoltaic materials due to their high-power conversion efficiency, and solar cells based on MAPbI₃ have reached a power conversion efficiency (PCE) over 25% [1]. The commercialization of this technology is hampered by the toxicity of lead (Pb); however, tin (Sn), which is also a group 14 element like Pb, forms similar crystal structures and is considered the most promising alternative.

Despite similarities in electronic properties between MASnI₃ and MAPbI₃, the photoelectric efficiency and stability of tin halide perovskites are limited by self-p-doping and tin oxidation [2]. It is essential to investigate the microscopic origin of these phenomena to propose solutions and promote the use of lead-free perovskite solar cells. In this work, a detailed investigation of the electronic and optical properties and thermodynamic stability and trapping activity of native defects in MASnX₃ is carried out, which is achieved using density functional theory (DFT) calculations. The findings from such investigations may lead to novel approaches to overcome the issues associated with tin halide perovskites, thereby promoting the widespread use of lead-free perovskite solar cells.

The results of defect energy calculations (Fig. 1) based on first-principles indicate that Sn vacancies and X-site interstitial atoms are easily formed among several defects in MASnX₃. Among them, MASnCl₃ is found to be less likely to form Sn vacancies, and is considered to be more stable than MASnBr₃ and MASnI₃ due to the stability of its formation energy and its tolerance factor (0.95) being close to that of ideal perovskite. X-ray absorption near edge structure (XANES) theoretical calculations show a small discrepancy between the XANES spectrum with Sn vacancies and that of the defect-free structure, whereas with interstitial X-site atoms, there is a clear discrepancy with the XANES spectrum of the defect-free structure. This may be due to the fact that the crystal structure around the interstitial X-site atoms is distorted, while the change in crystal structure due to the Sn vacancies is minimal.

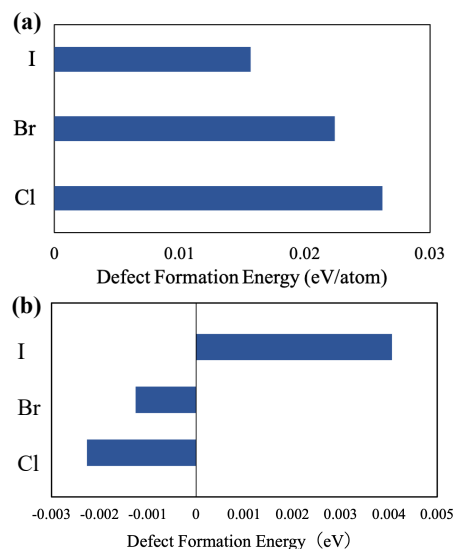


Fig. 1 The defect formation energy of (a) Sn vacancies and (b) interstitial X-site atoms in MASnX₃.

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Performance Optimization of Ge: Sn (1:1) Perovskite Solar Cells Using Doping Engineering

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Lead-free materials are rigorously explored as substitutes for environmentally friendly photo-harvesting applications. Germanium (Ge) as a replacement of lead forms perovskite structure with promising theoretical optoelectronic results. However, its practical application is hindered by low octahedral factor values (≈ 0.33). Conversely, tin (Sn) has demonstrated exemplary experimental and theoretical results as a lead replacement. In this study, we fabricated a Ge: Sn /1:1 perovskite film with an improved octahedral factor of ≈ 0.43 , to harness the excellent optoelectronic properties of Ge-Sn alloyed film.

As a first step, we devised a dimethyl sulfoxide (DMSO) free solvent system, as DMSO rapidly oxidizes GeI_2 and SnI_2 . X-ray diffraction pattern, UV-vis spectra, and photo yield spectra measurements confirmed the successful formation of Ge-Sn (1:1) crystal, fabricated using simple spin coating methods.

Subsequently, we fabricated Ge-Sn films on PEDOT:PSS/FTO and deposited C60/BCP/Ag layers sequentially using thermal evaporation to complete the solar cells fabrication. However, the photoelectric performance was limited due to poor solubility of GeI_2 . To address this, in the next step, we employed an additive engineering which enhanced the solubility of GeI_2 and subsequently reduced the nonradiative recombination. An enhanced efficiency 3.23 % (FF=0.61, open circuit voltage=0.53V, short circuit current density=10.03mA/cm²) was obtained. Figure 1 shows the maximum power point tracking (MPPT) testing inside N₂ filled glove box. At the end of 1000 seconds measurements, 85% of initial efficiency was maintained. The complete device fabrication process and role of additives pertaining to the device performance enhancements will be discussed in the conference.

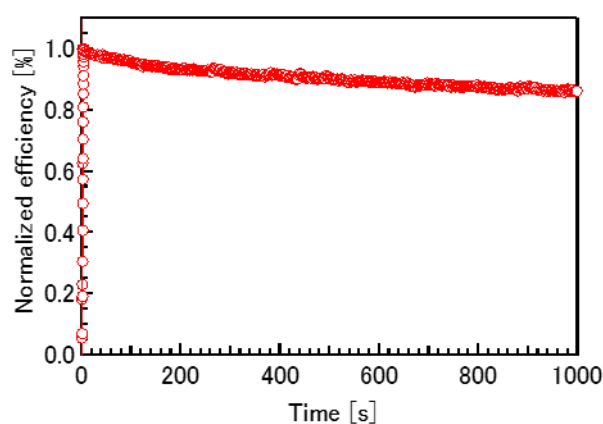


Figure 1: MPPT test of fabricated Sn-Ge perovskite solar cells

Resolving the Light and the Thermal Stability Issues in the Tin-Lead Perovskite Solar Cells by Manipulating the Carrier Selective Layers with Dopant and/or Passivation

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The investigations into the stability issues in the tin-lead (SnPb) based perovskite solar cells (PSCs) have been increasing as of lately while the performance reaching more than 24% in efficiency has been reported ¹. It is important to achieve excellent stability under prolong light illumination and thermal exposure above the room temperature for the SnPb PSCs to compete with existing solar cells. Various reports are available on the stability improvement such as the introduction of additives or dopants in the active layer of the SnPb PSCs; substituting or passivating the PEDOT:PSS hole transport layer with non-acidic materials such as carbazole based self-assembled monolayer ^{2,3}, substituting the silver electrode with metal copper or carbon derived materials and many others. The core improvement of the stability based on these studies pin-point to the ion migrations as the main culprit for the stability issues in the PSCs. Thus, reinforcing the carrier selective layers seemingly important in order to mitigate the migrations of ions across the SnPb PSCs. In this research, we will demonstrate the effects of incorporating the carrier selective layers of the SnPb PSCs with dopant and/or passivation layer on their light and thermal stabilities. The preliminary results showed the PCE improvement to more than 22% efficiency and overall solar cell parameters such as FF, Jsc and Voc; due to the decrease in shunting and enhance recombination resistance which correlated well with the reduced migration of ions under XPS investigation near the electron transport layer. The light and the thermal stability studies were conducted on the SnPb PSCs with modified carrier selective layers showed enhanced stability under prolong exposure to light and elevated temperature.

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