Kwansei Gakuin University
Report of Research Outcome

2025/01/08

To President

Department : Science and Technology
Position : Postdoctoral fellow
Name : Shengnan Duan

I report the outcome of the research as follows.

Name of the Fund/Program	□Sabbatical leave with grant □Sabbatical leave with no grant □KGU Joint Research □Individual Special Research ☒Postdoctoral fellow ※Please report by designated form as for "International Research Collaboration".
Research Theme	Charge Transfer Dynamics Study of Z-scheme Heterojunction based Solar Cells by Transient Absorption Spectroscopy
Research Site/Venue	Kobe Sanda Campus Building VII
Research period	2024/04/01 ～ 2025/03/31 （ 12 months）

◆ **Summary of the research outcome** （approx. 2,500 words）

Please write down the outcomes in detail regarding the research theme above.

Work 1: Investigating the Working Mechanism of Natural Photosynthesis-Inspired Solar Cells via Sub-Picosecond Transient Absorption Spectroscopy

The natural Z-scheme of oxygenic photosynthesis efficiently drives electron transfer from photosystem II (PSII) to photosystem I (PSI) through an electron transport chain, overcoming the lower energy levels of PSII. Drawing inspiration from this sophisticated mechanism, we developed a cascade bio-solar cell (CBSC) featuring a layered architecture that mimics the Z-scheme. In this design, chlorophyll derivatives (Chl) function as PSI analogs, while bacteriochlorophyll derivatives (BChl) serve as PSII analogs within the active layer. The resulting photocurrent, prominently observed in the near-infrared region, was confirmed by external quantum efficiency measurements. Sub-nanosecond transient

absorption spectroscopy revealed a prolonged charge transfer (CT) state from BChl to Chl ($Chl^-/BChl^+$ species) compared to the reverse direction ($Chl^+/BChl^-$ species). This asymmetry underscores a predominant electron flow from BChl (PSII analog) to Chl (PSI analog) under simultaneous excitation, effectively replicating the natural Z-scheme electron transfer pathway. These findings represent a major breakthrough in the design of bio-inspired solar cells, offering valuable insights into artificial photosynthesis systems and advancing photovoltaic theory and efficiency.

The related manuscript has been published at ChemSusChem, 2025, e202402588 (Impact Factor: 7.5), of which Shengnan Duan is the first author and Hideki Hashimoto is the corresponding author.

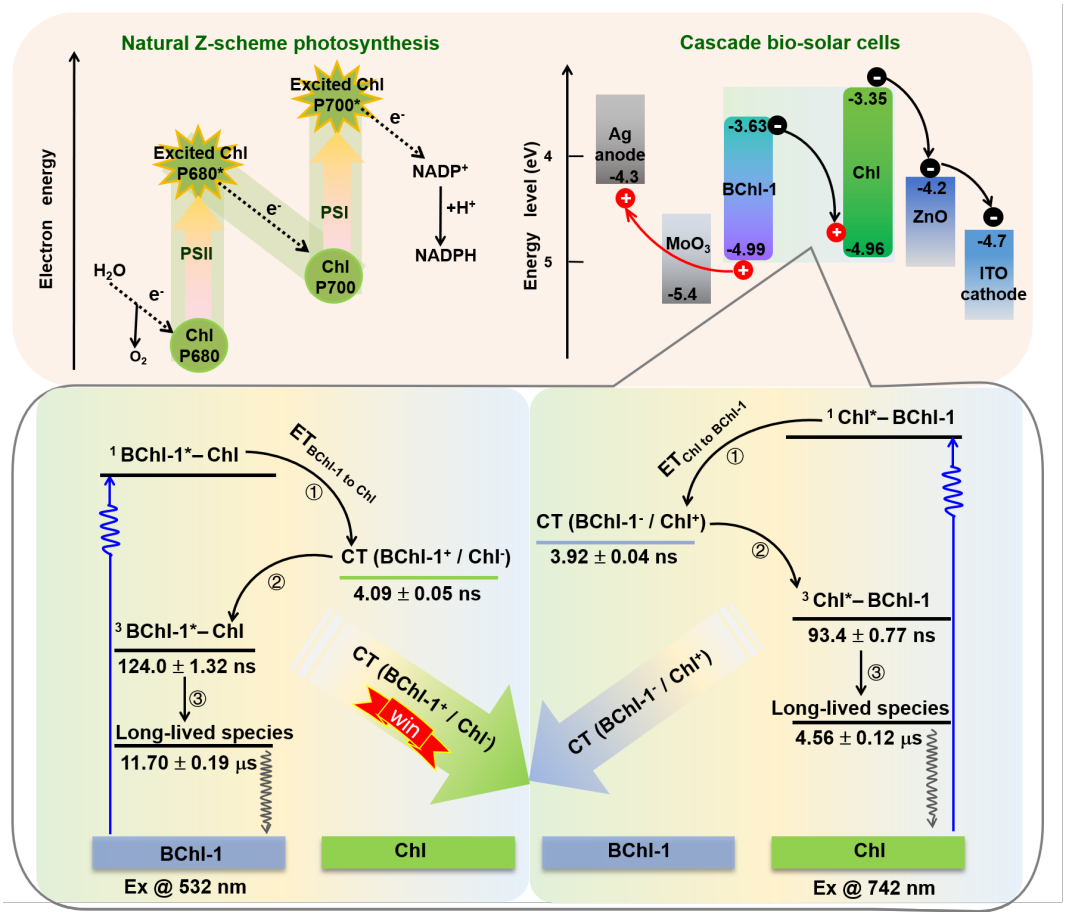


Figure 1. Schematic representation of natural Z-scheme photosynthesis and the bio-solar cells inspired by it, along with the energy transfer processes in the Chl/BChl-1 active bilayer investigated by sub-ps TAS spectroscopy.

Work 2: Unleashing the Potential of Bio-Based Additives: Semi-Synthetic Chlorophylls for High-Performance Organic Solar Cells

Chlorophylls (Chls), the most abundant natural pigments, are celebrated for their

exceptional optoelectronic properties and biocompatibility. In this study, we report high-efficiency, eco-friendly binary organic solar cells (OSCs) incorporating semi-synthetic chlorophyll derivatives, designated as Chl-1 and Chl-2, as "green" solid-state additives. These additives address the dual challenges of enhancing device efficiency and ensuring sustainability. The three-dimensional, semi-synthetic Chl derivatives optimize the molecular stacking and crystallinity of the active layer, inducing a favorable face-on molecular orientation and a denser crystalline structure. These structural modifications promote efficient exciton dissociation and charge transport, as validated by time-resolved femtosecond transient absorption spectroscopy. Consequently, the Chl-based devices achieve superior photovoltaic efficiencies of 19.01% for Chl-2 and 18.80% for Chl-1, outperforming the control binary devices (18.05%). This study demonstrates an innovative strategy for advancing the commercialization of wearable OSCs by integrating eco-friendly semiconductor materials. The findings provide a pathway to reconcile environmental sustainability with high-performance energy conversion, paving the way for greener, more efficient solar technologies.

The related manuscript is currently submitted to a high-impact international journal.

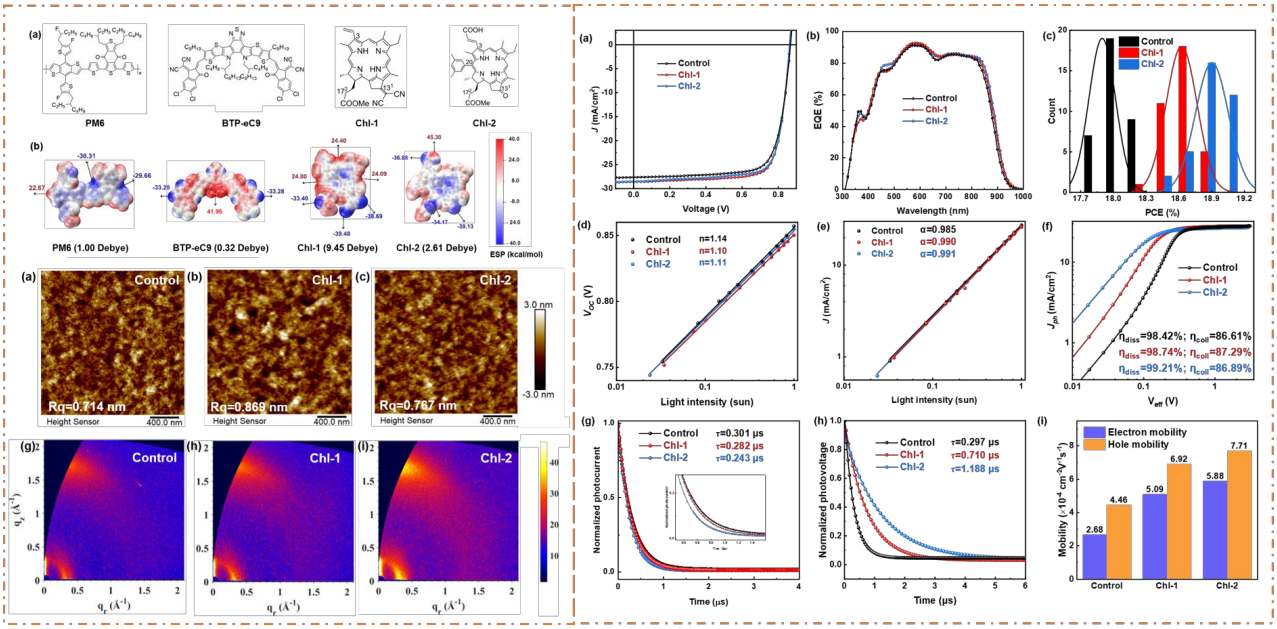


Figure 2. Partial data proposed from this work.

Work 3: Natural Chlorophyll-*a* and Its Derivative as Bio-Additives for Efficient and Biocompatible Organic Solar Cells

Additive-assisted regulation of donor and acceptor domains is a well-established strategy to enhance the photovoltaic performance of existing organic solar cells (OSCs).

However, identifying efficient, stable, non-toxic, and low-cost biological materials to replace traditional halogen-based additives remains a critical challenge. In this study, we employed natural chlorophyll-*a* (Chl-*a*) and its derivative (Chl-*s*) as bio-additives to optimize the morphology and molecular stacking of the active layer in OSCs. The incorporation of Chl-based additives facilitated the fine-tuning of the donor-acceptor microstructure network, resulting in a significantly improved power conversion efficiency (PCE) of 19.06%, compared to 17.97% for the control device. These results demonstrate the potential of eco-friendly and biocompatible chlorophyll derivatives as effective bio-additives for enhancing the photovoltaic performance of OSCs. **The ongoing work is now focused on data collection, and the findings will be compiled into a manuscript for submission in the near future.**

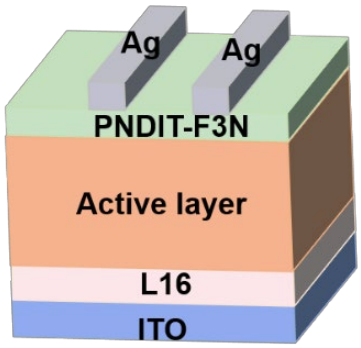


Figure 3. Device structure of the OSCs incorporating the natural Chl-a and its derivative as additives.

Work 4: Successful Approval of the High-End Foreign Expert Introduction Program of China

We are pleased to announce the successful application and approval of the High-End Foreign Expert Introduction Program of China, with Prof. Hashimoto as the invited expert (Grant No. H20240882). The program has provided a total funding of 400,000 RMB (approximately 8.6 million JPY), which will support the ongoing scientific collaboration between Prof. Hashimoto and myself. This special funding represents a significant opportunity to strengthen our joint research efforts. I am confident that, with this continued support, we will achieve even more impactful and meaningful results in our collaborative work.

基本信息（系统编号：110000215020248009）

项目类型	国家外国专家个人类项目(H类)	项目名称	高效率人工光合成仿生太阳能电池的工作机理及其商用化研究
资助类型	国家资助	项目状态	国家批复通过
项目编号(立项后系统生成)	H20240882 国家立项	学科	理学-物理学
专业领域	数理科学	项目关键字	成渝经济圈,碳达峰碳中和,新能源,中日合作
项目起止日期	2024-01-01至2025-12-31		
创建时间	2024-07-19 09:37	更新时间	2024-09-02 14:57

Figure 4. The approval information of High-end Foreign Expert Introduction Program of China (In Chinese version).

Work 5: Attendance at the 24th International Conference on Photochemical Conversion and Storage of Solar Energy (Hiroshima, Japan), Serving as Session Chair, and Winning the Oral Presentation Prize

I attended the 24th International Conference on Photochemical Conversion and Storage of Solar Energy in Hiroshima, Japan, where I served as a Session Chair. During the conference, I was honored to receive the Oral Presentation Prize for my presentation.

Session IPS-24 / ICARP2024

Oral Presentation | Artificial photosynthesis and natural photosynthesis

Tue. Jul 30, 2024 10:30 AM - 12:15 PM JST | Tue. Jul 30, 2024 1:30 AM - 3:15 AM UTC Room E(Cosmos-2)

[30amE-Oral] "Meso-Hierarchy" Session

Chair:Ryu Abe(Kyoto University), Shengnan Duan(Chongqing University of Posts and Telecommunications&Kwansei Gakuin University)

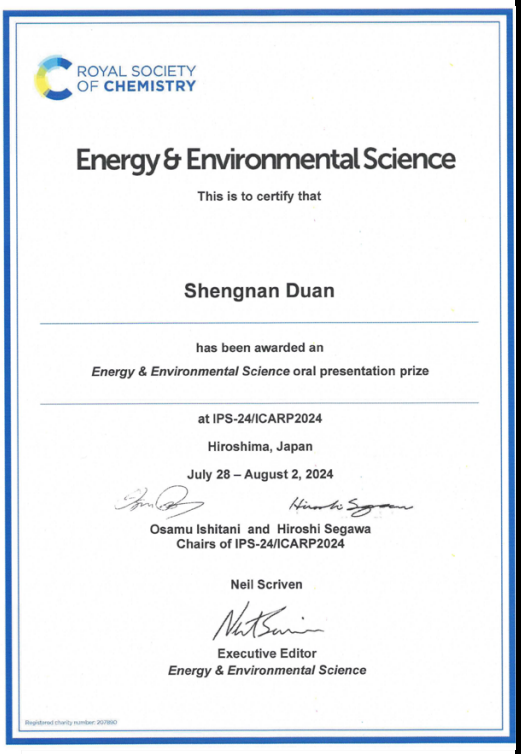
Session Chair

10:30 AM - 11:00 AM JST | 1:30 AM - 2:00 AM UTC
[2E-01-KL]
Construction of Molecular Architectures for High-Yield Singlet Fission
*Taku Hasobe[1] (1. Faculty of Science and Technology, Keio University (Japan))

11:00 AM - 11:25 AM JST | 2:00 AM - 2:25 AM UTC
[2E-02-IL]
Energy transfer in quantum dot-organic molecule systems toward effective utilization of solar energy
*Sadahiro Masuo[1] (1. Kwansei Gakuin University (Japan))

11:25 AM - 11:50 AM JST | 2:25 AM - 2:50 AM UTC
[2E-03-IL]
Theoretical study of charge photogeneration dynamics in organic photovoltaics
*Takatoshi Fujita[1] (1. National Institutes for Quantum Science and Technology (Japan))

11:50 AM - 12:15 PM JST | 2:50 AM - 3:15 AM UTC
[2E-04-IL]
Time-resolved spectroscopic tracking of exciton diffusion dynamics in mesoscale molecular assemblies
*Hikaru Sotome[1], Sho Takahashi[2], Shiki Yagai[2], Hiroshi Miyasaka[1] (1. Osaka University (Japan), 2. Chiba University (Japan))



ROYAL SOCIETY OF CHEMISTRY

Energy & Environmental Science

This is to certify that

Shengnan Duan

has been awarded an

Energy & Environmental Science oral presentation prize

at IPS-24/ICARP2024

Hiroshima, Japan

July 28 – August 2, 2024

Osamu Ishitani and Hiroshi Segawa
Chairs of IPS-24/ICARP2024

Neil Scriven

Executive Editor
Energy & Environmental Science

Figure 5. the Chair information and Oral Presentation Prize of IPS-24 (Hiroshima, Japan)

Deadline : Within two months after finishing the research period.

Sabbatical leave with grant: Submit this report to President with confirmation by the dean of school you belong to.

※Postdoctoral fellow is required to submit this report with confirmation by the dean of graduate school before the end of employment period.

Where to submit : Organization for Research and Development and Outreach (NUC)

◆We put this report on the web of KGU. If there is any problem about it because of difficulties on your research, please let us know.