ASPIRE League Research Grant 2014 (Type1) Project

Principal Researcher	Name	**Yuji Wada**
	Department and graduate school(institute)in Tokyo Tech	Department of Applied Chemistry, Graduate School of Science and Engineering
	Position	Professor
Co-researchers	HKUST	Shihe Yang, Professor, Department of Chemistry
	KAIST	Byungha Shin, Assistant Professor, Department of Materials Science and Engineering
	NTU	Nripan Mathews, Assistant Professor, Department of Materials Science and Engineering
	Tsinghua	Hong Lin, Professor, School of Materials Science and Engineering
Subject of the research project		**Creation of Ideal Interfaces of Organic-Inorganic Hybrid Solar Cell Leading to Commercially-applicable High-throughput Fabrication Process for Flexible Device**
Summary of the research project		The mesoscopic organic-inorganic hybrid solid-state solar cell (MS-cell) based on combining organic and inorganic semiconductors (SC) is a highly attractive subject due to its high conversion efficiency, >15% (lab-scale), and ease of production based on printable processes. The challenges in developing this solar cell are proposed as 1) construction of ideal interfaces for more efficient charge transfer, 2) efficient photon-absorber in near-IR (NIR) region for high efficiency, 3) novel production technology for high-throughput manufacturing, and 4) alternative semiconducting and photon-absorbing materials to replace Pb-derivatives. The results of the preceding collaborative research on dye-sensitized solar cells (DSSCs) in the laboratories of synthetic organic chemistry, materials sciences, and physical chemistry in our department will be extensively applied to the MS-cell system that shares common structures with DSSCs in order to solve the problems of 1 and 2. In addition, the analytical techniques of charge transfers at interfaces established in the DSSC area can also be applied to further understanding those of the MS-cell. The principal

Summary of the research project	researcher's pioneering work on microwave (MW) chemistry can also be applied to the construction of the high-throughput process of flexible solar cell devices for commercialization as problem 3. We would invite collaborators for the three subjects in this project as listed below, 1) printable perovskite-based hybrid SC without toxic compounds, 2) computational chemical simulation of the organic-inorganic hetero-interfaces by means of quantum chemistry and molecular dynamics, and 3) microwave-processing for fabrication. The alternative printable photon-absorbing perovskite-based hybrid SC using non-toxic and naturally-abundant materials, such as Sn, Cu, etc., is highly desired, since the conventional MS-cell is primarily composed of $(R\text{-}NH_3)PbX_3$ (R= hydrocarbon and X=halogen) containing the harmful heavy metal, Pb, which is a large obstacle for commercialization of MS-cells. The collaborator is supposed to provide optimized deposition conditions and photon-electronic properties. The materials are assembled with our nanostructured oxide SC scaffold. The interfacial charge transfer properties are examined to provide feedback for further material development. The second collaborator is in charge of the simulation of interfacial morphology between the hole conductor and the dye-sensitizer at the interfaces with quantum chemistry and molecular dynamics. The simulated interfacial information is feedbacked for designing dye-sensitizers. The third collaborator is in charge of the development of MW technologies for fabrication of the cells. The principal researcher (PR) has over 20 years experience with chemical and physical research in DSSC and MW chemistry, which is valuable in developing the MS-cell. Additionally research collaboration in DSSC at Tokyo Tech has been proceeding for 4 years, which is a large advantage for the quick start-up in this new research field of MS-cells. A new collaboration with ASPIRE league members would facilitate the diversity needed to generate novel innovations for a realistic MS-cell with the potential for large-scale commercialization.