Fiscal Year 2018, Tokyo Institute of Technology ASPIRE League Research Grant

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Selected Research Project for Type 1 in FY2018

Principal Researcher	Name	**Takafumi Ueno**
	School at Tokyo Tech	School of Life Science and Technology
	Position	Professor
Co-researchers	HKUST	ZHU Guang, Professor Division of Life Science
	KAIST	Yoon Sung Nam, Associate Professor Department of Materials Science & Engineering,
	NTU	Sierin LIM, Associate Professor School of Chemical and Biomedical Engineering, Kelin Xia, Assistant Professor School of Physical & Mathematical Sciences,
	Tsinghua	Diannan Lu, Associate Professor Department of Chemical Engineering
Subject	Functional Design of Protein Cage for Sustainable Bio-nanomaterial	

Summary of the research project

Protein assemblies have recently become recognized as potential molecular scaffolds for applications in materials science and bio-nanotechnology. Efforts to design protein assemblies for construction of protein-based hybrid materials with metal ions, metal complexes, and nanomaterials now indicate a growing field with a common aim of providing novel functions and mimicking natural functions. However, the important roles of protein assemblies in sustainable materials science have not been systematically investigated and established.

Protein cage is one of the most useful scaffolds among protein assemblies with nano-sized structures, such as tube, wire, and two-dimensional array, because the cage has a various range of diameter from several to hundreds nm, and can be conjugated with natural and synthetic functional molecules on both the inside and outside surfaces. Many researchers reported functionalization of protein cages for the broad range of applications and implications focusing on the medical and biotechnology sectors. However, there is a limitation on development of drug delivery and imaging reagent due to low stability to conjugate various composites involving inorganic materials. Thus, highly robust protein cages are required to encapsulate and display inorganic materials with bionano functions, such as drug delivery and imaging.

We therefore propose to design and construct new types of sustainable protein cages conjugated with inorganic compounds for medical and bionano-applications. Ferritin (Fr), which plays the role of an iron storage protein, is known to accommodate various metal ions/complexes and is suitable for catalytic reactions conducted in an aqueous medium. From a protein engineering point of view, the effective preparation, yield, and stability make the Fr cage suitable for use as molecular templates to accumulate metal ions, complexes, and nanoparticles for construction of sustainable biomaterials to deliver metal drug and metal imaging reagents, such as gold and silver nanoparticles, and gadolinium complexes, into living cells. The accumulation of the inorganic compounds with desired size, number and position in the Fr cage is required for the accurate functions promoted in living cell. Thus, in the research project, we pursue the following objectives to establish the new research field of sustainable bio-nanomaterials :

(1) Computational design of the Fr cage

(2) Incorporation and preparation of inorganic materials in the Fr cage and surface modification of the composite

(3) Evaluation of the functions toward medicinal and biomaterial applications

Principal Researcher	Name	**Tsuyoshi Michinobu**
	School at Tokyo Tech	School of Materials and Chemical Technology
	Position	Associate Professor
Co-researchers	HKUST	Mansun Chan, Professor Department of Electronic and Computer Engineering
	KAIST	Bumjoon Kim, Professor Department of Chemical & Biomolecular Engineering
		Steve Park, Assistant Professor Department of Materials Science and Engineering
	NTU	Qichun Zhang, Associate Professor School of Materials Science and Engineering, School of Physical and Mathematical Sciences
	Tsinghua	Guifang Dong, Associate Professor Department of Chemistry
Subject	Organic thin film devices based on narrow band gap semiconducting polymers	

Summary of the research project

Narrow band gap semiconducting polymers, implemented in mobile displays, radio frequency identification tags, electronic papers and skins due to their designable synthesis, solution-processability, high thermal stability, and mechanical flexibility, are important materials for future electronic devices. In the past decade, remarkable achievements have been made in polymer thin film transistors (TFTs) with high carrier mobilities over 10 $cm^2 V^{-1} s^{-1}$, which are competitive with or even surpassing the benchmark mobility of amorphous silicon semiconductors.

In order to further increase the carrier mobilities of polymer TFTs, three important polymer design principles are proposed. First, conjugated coplanar backbones with a low conformational disorder must be developed. This enables the formation of short π–π stacking and strong intermolecular interactions in the thin film states. Second, side chain engineering is a powerful tool in increasing the polymer solubility into organic solvents and crystallinity in the thin film states. Third, the introduction of heteroatoms into the π-conjugated backbones results in fine-tuning of energy levels and intermolecular interactions. With these design guidelines in mind, novel semiconducting polymers based on benzobisthiadiazole (BBT) units have been developed by our group. The TFTs based on BBT polymers showed very high mobilities reaching 3.2 $cm^2 V^{-1} s^{-1}$, tunable polarities, and remarkable air stability. Grazing-incidence wide-angle X-ray scattering (GIWAXS) studies of the thin films revealed the importance of the polymer crystallinity and packing orientations. In the ASPIRE League collaborations, these polymers will be applied to high-performance transistors including complementary metal-oxide-semiconductor (CMOS)-like devices, all-polymer solar cells, carbon nanotube (CNT) composite devices, nonvolatile memories, and multi-layer photodiodes. Furthermore, flexibility and mechanical toughness or self-healing properties would be given to these devices.