Harnessing the Potentials of Organic Photofunctional Materials for Energy, Environment and Health

SHYAM S. PANDEY
(Professor)
Graduate School of Life Science and Systems Engineering,
Kyushu Institute of Technology

Moving with the philosophy of the Graduate School of Life Science and Systems Engineering (LSSE), we are dedicated to interdisciplinary research aiming toward providing an amicable solution for the intriguing issues about energy, environment and health. Our focus has been directed towards exploring the wonderful world of NIR sensitive organic photofunctional materials for their applications in the area of energy harvesting, organic electronic devices and sensing. We strive for multi-disciplinary research from theoretical material design and development to their implementation for low-cost efficient devices with the least burden on our environment. This allows students to acquire a way of analytical thinking, environmental consciousness and uniquely interdisciplinary research.

Focusing on the Energy, Environment & Health to support SDGs!

Amongst the targets of sustainable development goals (SDGs), amicable solutions for intriguing issues like energy, environment and health are inevitable. Research focus in my laboratory has been directed towards **(1)** design and development NIR sensitive novel photofunctional materials based on combined theoretical and experimental approaches, **(2)** development, improvisation and visualization of cost-effective, large area and oriented thin films and **(3)** applications of the newly designed functional materials. The main application areas in focus are (a) next-generation cost-effective dye-sensitized solar cells (DSSCs), (b) Low-cost and energy-efficient organic electronic devices, and (c) Sensing for the monitoring of the environment and health as outlined in **Fig. 1**. Apart from design, synthesis and materials characterization, students will be able to challenge the diverse application potentials as indicated in item (3).

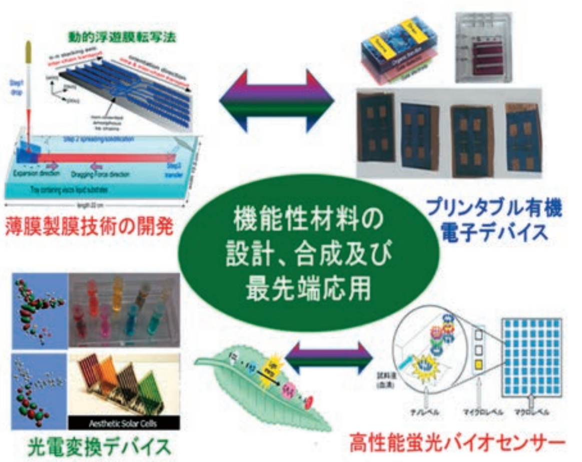

Fig. 1. Outline of the Inter-disciplinary research carried out in my laboratory.

Development of NIR-sensitive photofunctional materials

The development of NIR sensitive photofunctional materials is one of the main targets of functional materials development in my laboratory. Such materials have tremendous technological potential in enhancing the overall photoconversion efficiency (PCE) of the next-generation organic solar cells, flexible low-cost and low-energy consuming organic electronic devices and efficient sensors/biosensors. A target functional material for desired application must fulfil some requisite criteria in terms of energetics, optical properties and energy bandgap etc. for their suitability. In our laboratory, we utilize state-of-art quantum chemical calculations using the Gaussian program for reliable prediction of energetics and optical properties. Utilizing experimentally designed squaraine class of NIR dyes (>150), we have demonstrated an excellent correlation between the experimental and corresponding theoretically predicted results with only an error of 0.1 eV and 0.06 eV for energetics and absorption maximum/optical band gap, respectively.

Low-cost and beautiful energy harvesting via DSSCs

DSSCs, a mimic of natural photosynthesis, got huge attention owing to lost-cost fabrication, lightweight, flexibility, vibrant colour and transparency. This makes them ideally suited for building integrated photovoltaic (BIPV) applications. State-of-art techno-scientific innovations for DSSCs after their inception led to the demonstration of nearly quantitative photon harvesting mainly in the visible wavelength region surpassing the PCE of amorphous silicon. PCE>15% is a bottleneck for commercialization and utilization of NIR dyes with intense light absorption in the NIR region (>700 nm) is inevitable to achieve this goal. A PCE of 5%–7% mainly in the NIR wavelength region is expected a play a dominant role in achieving this target. Our laboratory is involved in the R&D of different aspects of DSSCs such as solid-state, flexible, transparent and bifacial with emphasis on the utilization of newly designed NIR dyes. We have recently developed brilliant green coloured NIR dye (**SQ-140**), mainly harvesting photons in the NIR region with a PCE of 6%. Transparency and efficiency are inversely proportional and average visible transparency (AVT) >30% is desired for good visual perception. Recently a PCE of 4–7 % with AVT of 40–60% has been demonstrated using silicon solar cells with micro-slits and holes. Utilizing a yellow coloured commercial dye in combination with our newly SQ-140 dye, we recently demonstrated transparent DSSCs with PCE and AVT of 5.5 % and >35%, respectively as shown in **Fig. 2**.

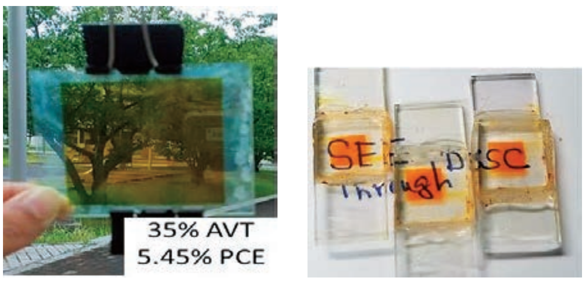

Fig. 2. Transparent DSSC using a dye cocktail of visible yellow and green dyes.

Research focuses on the development of organic electronic devices

Semiconducting polymers possess excellent robustness in terms of flexibility and stretchability, making them capable of coating complex surfaces expanding the scope of microelectronic devices. High throughput and fabrication of large-area oriented thin films are some of the intriguing issues for the realization of the large-area and flexible organic electronic devices. Spin coating is the most widely used method for thin-film fabrication but issues like huge material wastage (>90%), difficulty in multilayer coating and molecular orientation. In my laboratory, research focus in the area of organic electronics is directed towards the design and development of high-performance photofunctional organic semiconductors, fabrication and characterization of directionally large area oriented thin films and utilization of such thin films for fabrication of high performance and flexible organic electronic and optoelectronic devices. In the area of thin-film fabrication, we are involved in the development and improvisation of solution-processable thin film fabrication methods like dynamic floating-film transfer method (FTM) and Friction Transfer techniques along with the swift, simultaneous and quantitative visualization of uniformity and molecular orientation. FTM is a simplified version of the famous and old Langmuir-Blodgett film fabrication method, where dragging viscous force of the orthogonal liquid substrate to spreading organic semiconducting polymer ink imparts simultaneous orientation, which is shown in **Fig. 3**. Contrary to the conventional spin-coating method, FTM processed thin films are highly material-efficient (>90% material use) and >25 times cost-effective. Thanks to the isolation of thin-film formation followed by its transfer layer-by-layer coating of large-area prefabricated films not only provides the opportunity to make complex heterostructures but also offers the separate control of the thin-film morphology independent of the substrate's surface morphology. We have not only demonstrated the fabrication of large-area (>40 cm^2) uniform and oriented thin films by FTM but

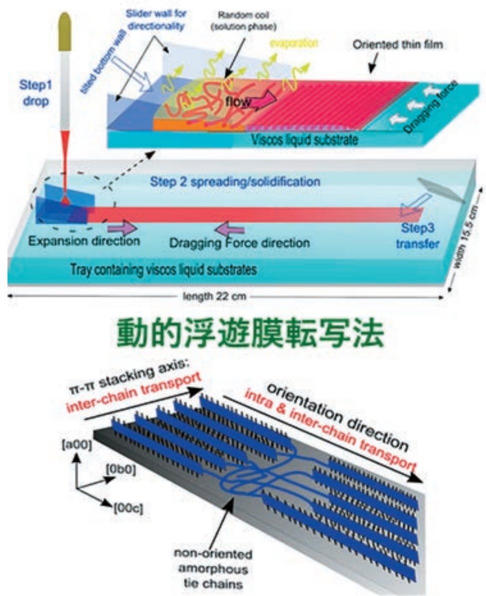

Fig. 3. Schematics of thin film fabrication and mechanism of orientation under FTM (top) and assembly of oriented semiconducting polymers in FTM thin films (bottom)

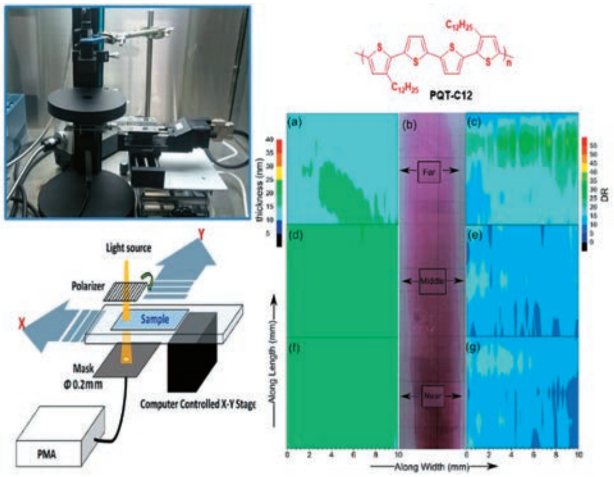

Fig. 4. Schematics of our 2D positional mapping system (left) and result of mapping of distribution in thickness and orientation in the large area and oriented thin film of conjugated polymer PQT-C12 prepared by FTM (right).

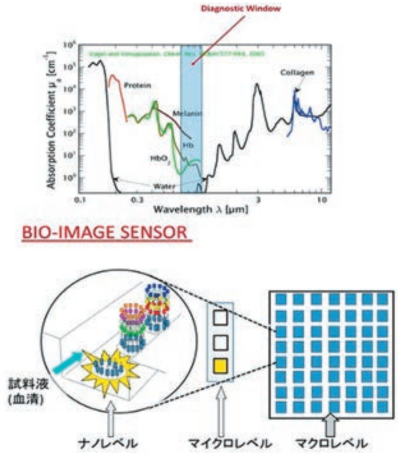

Fig. 5. Absorption spectra of different components of biological matrix (top) and schematic representation of our proposed Bio-image sensor.

also demonstrated the applicability of this method utilizing a variety of organic semiconducting polymers. Apart from the facile fabrication of large-area thin films, their swift characterization to ascertain the uniformity is highly desired. To address this, we have also developed a 2D-positional mapping system for swift characterization of large-area thin-films for the high throughput and simultaneous mapping of the distribution in the thickness and molecular orientation as schematically shown in **Fig. 4**. Incorporation of the computer-controlled XY-stage controller, a polarizer and simultaneous detection of all output wavelengths by 1056 CMOS detectors allows swift and simultaneous mapping of thickness and molecular orientation. The reliability of the measurement system was successfully validated by a standard double beam spectrophotometer and large area thin films of conjugated polymers fabricated by different methods such as spin-coating, friction transfer and FTM. Utilizing highly oriented thin films of PBTTT-C14, a liquid crystalline solution-processable organic semiconductor, we fabricated an organic thin-film transistor with field-effect mobility of 1.24 cm^2/Vs (surpassing amorphous silicon), which is one of the highest mobility reported for this class of organic semiconductors. Development of Biodegradable organic electronic devices utilizing the design and development of biodegradable polymers and device elements to address the intriguing issue of the electronic garbage disposal for a clean environment is our future target.

Research focus in the area of sensing/biosensing

My laboratory is also involved in the R&D of high-performance sensors/biosensors for monitoring the environment and health conditions. By the fusion of wavelength-tunable flexible organic photodetectors and fluorescence resonance energy transfer (FRET) enabled fluorescence biosensors, our final goal is to develop a high-performance bio-image-sensor for simultaneous and multi-model analysis of the biological elements for early disease diagnosis as shown in **Fig. 5**. The main focus is directed toward tunable fluorescence detection in the NIR wavelength region of 650 nm–900 nm (diagnostic window). In this region fluorescence of biological sample matrices like tissue, blood and urine have ultra-low auto-fluorescence allowing highly sensitive signal detection and avoiding prior sample processing as commonly being done in analytical testing laboratories. Therefore, the development of such bioimage sensors will lead to the realization of efficient point-of-care testing devices, especially for the developed and ageing societies. Research in the area of utilizing NIR dyes to design NIR dye-Peptide FRET system based fluorescence probes and its fusion with the wavelength-tunable photo-detection system to realize highly efficient bio-image sensor is being actively carried out in my laboratory.