7-3　物質分子科学研究領域の評価

7-3-1　Ching W. Tang 外国人運営顧問

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Evaluation report by Ching W. Tang

With introduction through Professor Masahiro Hiramoto more than a year ago, I was invited by Director General Maki Kawai to visit with IMS and to serve as its Foreign Council Member. The actual visit, planned for the same year, did not happen due to the COVID-19 pandemic. Instead, we held a virtual meeting—through Zoom on May 6 and 7, 2021—in which I heard a series of presentations by the faculty of the Department of Materials Molecular Science on their ongoing research programs, followed with discussions. I was also given an overview of the status of UVSOR—the synchrotron radiation facility at IMS. Professor Maki began the two-day meeting with a general review of IMS.

As a task for Foreign Council Member, I was asked to provide an assessment of the research activities in the Department of Materials Molecular Science and advice on its future directions. I must admit it is a difficult assignment for a single individual given the very wide range of research disciplines undertaken by the Department's principal investigators and their associates, and the lack of expert knowledge on my part in some of these disciplines. Below I will attempt to evaluate as objectively as possible the research activities of individual principal investigators from what I learned in our meetings and their published materials. Understandably, in disciplines outside of my own expertise I can only provide a general impression, which may not necessarily reflect an accurate assessment of the PI's work or accomplishments. Where possible, I will make recommendations on future directions.

Remarks on Individual PI's research activities:

Yokoyama, Toshihiko

Research field: Spectroscopic methods for material and surface science.

Recent focus: X-ray magnetic circular dichroism (XMCD); ambient pressure hard x-ray photoelectron spectroscopy (HAXPES); time-resolved spectroscopic measurements using x-ray.

Remarks: I was truly impressed by Yokoyama's work on applying HAXPES for in situ analysis of chemical reactions in PEFCs during operation, and on understanding of the oxidation and reduction processes of the Pt electrodes and the PEFC degradation involving the poisoning of the Pt nanoparticles due to specifically the adsorption of the S anionic species. This work demonstrated that highly sophisticated scientific tools such as HAXPES are not only essential in broadening the fundamental knowledge in surface sciences, but also can provide specific information to help advance practical applications such as PEFCs.

Sugimoto, Toshiki

Research field: Surface and Interface Science.

Recent focus: Study of the physics of interfacial water using nonlinear optics; Surface engineering of photocatalytic water activation.

Remarks: Sugimoto's group studied, with SFG—a nonlinear optics technique, the orientation ordering of water molecules of ice films on Pt(111) and Rh(111). The water molecules were found ordered at the Pt(111) interface but disordered at the Rh(111) interface, which induced epitaxial growth of ice films on Pt and disordered growth on Rh. The finding is no doubt scientifically interesting and has provided a deeper understanding of the physicochemical property of water/solid interfaces. The group also published work on photocatalysis of water for hydrogen generation. However, currently there seems to be a lack of correlation between the fundamental study in understanding the water/solid interfaces and their relevance in making use of such findings to advance practical systems such as photocatalysis.

Hiramoto, Masahiro

Research field: Organic semiconductor materials and devices.

Recent focus: Organic solar cells, up-conversion devices, doping in organic semiconductors.

Remarks: The 2019 APL paper from Hiramoto's group on organic photovoltaic cells (OPVs) is noteworthy. It shows that the open-circuit voltage (V_{oc}) and fill factor (FF) in planar heterojunction OPVs can be remarkably improved with the use of highly crystalline organic semiconductors as both donor and acceptor. The V_{oc} and FF values are among the highest of photovoltaic devices based on either organic or inorganic semiconductors! Furthermore, the paper suggested the charge carrier recombination is via direct interband transition rather than through deep traps, the reason underlying the high V_{oc} and FF values. However, the short-circuit current is low and the overall power conversion efficiency of these crystalline OPVs is inferior compared to what has been achieved in the more conventional bulk heterojunction OPVs. This problem—due to the limitation of exciton diffusion length in organic semiconductors—has been an outstanding issue related the geometry of the planar heterojunction OPVs. Clearly, further works will need to be done to further improve the exciton diffusion length, via perhaps further increase in the carrier mobilities in the crystalline organic semiconductors.

The field of OPV, however, has been largely overshadowed by the emergence of perovskite-based solar cells in the last decade, even as the various PV technologies have matured, and the PV market has grown rapidly in recent years with 100+ gigawatts installation annually. It calls into question whether OPV devices, even if successfully developed, will ever compete with Si-based or other more developed PV technologies for electrical power generation in a significant scale.

Recent work from Hiramoto's group on up-conversion devices represents a need to develop novel organic electronic devices of practical functionality.

Nishimura, Katsuyuki

Research field: Solid-state NMR.

Recent focus: Development of solid-state NMR probe; structural characterization of super-molecular and bio-molecular materials.

Remarks: Since I have little knowledge of solid-state NMR, it would be inappropriate for me to make specific comment on Nishimura's work. From his presentation and the list of his publications, I gathered that he collaborated successfully with researchers outside of IMS to use solid-state NMR as a tool to elucidate molecular structures of a range of materials. An example he described in detail is the characterization of some insoluble fibrils in Amyloid β protein and of the pathways of their formation, which are important in understanding the origin of Alzheimer's disease, and I found it quite fascinating.

Kobayashi, Genki

Research field: Ion conductive materials, energy storage/conversion devices.

Recent focus: Characterization and application of H^- conductive oxyhydrides.

Remarks: Kobayashi group's research involved synthesis of novel metal oxyhydrides with an aim of achieving high H^- conductivity.

Superionic H^- conductors with a conductivity of ~10^{-1} S/cm has been obtained with BLHO class of materials at high temperatures. Potential applications include hydrogen storage, fuel cells, *etc*. A future work is aimed at achieving high conductivity at low temperature. Kobayashi is taking a non-conventional path to develop ionic materials for electrochemical devices with a strategy that is based on a deep understanding of structure–property relationship of a range of H^- compounds. Although the odds of a practical breakthrough remain high, the scientific undertaking is rational and methodical.

Yamamoto, Hiroshi

Research field: Organic electronics, OFET, spintronics

Recent focus: Mott transitions in organic crystals and related superconducting transistors

Remarks: Yamamoto group's research was focused on FETs (or OTFTs) based on insulator-to-metal Mott transition, where the FET switching is controlled by the insulator-to-metal phase transition either with light, electric field, or mechanical strain. The organic material of interest is $(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$ (κ-Br), a prototypical organic crystal well known for its superconductivity. The observed FET phenomena are interesting from the standpoint of basic molecular science, but as switching devices, the κ-Br Mott-transition type FETs are unlikely to be of practical use due to 1) performance limitation and insufficient differentiation over conventional FETs, 2) scalability of the organic crystal size in general, 3) operability only at super low temperatures, and 4) uncharted demand for all organic-based FETs. However, I believe it is certainly useful to adopt various device structures, such as FETs, as a tool for probing the fundamental properties of molecular materials with an aim for future applications—such as quantum devices as proposed by this group.

Kera, Satoshi

Research field: Surface science; Angle resolved ultraviolet photoelectron spectroscopy

Recent focus: Electronic states of functional organic materials

Remarks: Kera's presentation "Impacts of Low Dimensionality on Electronic States of functional Materials" detailed the progress and challenges of assessing the electronic states of organic-based, soft materials using synchrotron-light-source based photoelectron spectroscopy. While there is no doubt about the rich functionality found in organic materials, but fully understanding the electronic states and correlating them to observed electronic properties in organic-based devices such as OLED and OTFT are still work in progress after decades of investigation, as Kera pointed out. I am very impressed by his work on probing the electron–phonon coupling in rubrene crystals using ARUPS and the finding that the e–ph coupling has direct impact the hole mass and its transport in rubrene. His future research aiming at investigating the electronic states beyond the energy space to momentum space and from spectroscopy to imaging represents a huge leap in scientific scope and depth. It also raises the question of impact—how important is the probe into the fine features of electronic states of "soft" matters for further enhancement of their functionalities and device applications? As is the case for most fundamental scientific investigations, relevance is a tough call at a particular moment of time.

Matsui, Fumihiko

Research field: Synchrotron-radiation photoelectron spectroscopy and imaging

Recent focus: Photoelectron momentum spectroscopy

Remarks: Matsui's group is charged with the development of new photoelectron instrumentation that will "Open up a new trend of electron spectroscopy at IMS" in conjunction with the BL6U beamline of the UVSOR facility. From his presentation, which I must admit I could barely comprehend, I understood that he is on track to develop one of the world's most sophisticated photoelectron momentum microscope at IMS and ready to undertake a range of exciting experiments with the new tool. It seems to me the work of Matsui and Kera are highly complementary, an attribute to the strength of IMS in the development of photoelectron instrumentation with an inhouse UVSOR facility, and its utilization particularly in material characterization.

UVSOR III

Synchrotron radiation facility at IMS

Remarks: Director Kera gave an overview of the UVSOR—a synchrotron radiation (SR) facility, including a brief history, the current capabilities and operation, and a vision for the future. There is no doubt UVSOR in its various versions, has served the need of IMS and the research communities in Japan and around the world since its installation 37 years ago. Although it is one of the oldest among the more than 10 SR facilities in Japan, it appears that its upgraded version, UVSOR III, remains one of the best SR in providing VUV and soft X-ray beams with the highest resolution, making it particularly useful for chemical analysis—thus the realization of the "Chemical Machine" coined by the renowned former Director General H. Inokuchi. The highly accomplished work of Yokoyama, Kera, Matsui and many others from IMS would not have been possible without UVSOR. Charting the future of UVSOR may be more difficult, given the availability of newer and more modern SR facilities in Japan and elsewhere, and the usual constraint of funding in running a large dedicated capital-intensive facility. With continuous innovations in analytical capabilities for a wide range of research disciplines as demonstrated by the UVSOR team, and serving both academic and industrial laboratories, particularly in materials science, I believe UVSOR can carved out an area of excellence among the SR facilities and remain a vital and innovative scientific center for many more years to come.

Department of Materials Molecular Science

Remarks: The Department is relatively small in faculty size, as is the case for all IMS Departments. Yet, with 5 full-time faculty and a few others with cross appointments, the research disciplines are rather diverse with focus tilted more towards fundamental than applied research and emphasis on analytical and structural characterization of materials or material systems. Noticeably absent is material synthesis with exception of Kobayashi's activities on the development of oxy-hydride materials for ionic transport. Centered on electronic devices are activities from Hiramoto and Yamamoto's groups, with the former focused on developing efficient organic photoelectronic devices, including solar cells, and the latter on devices exhibiting unusual behaviors, such as superconductive FETs. It appears that the Department, as is, does not have the critical mass in each of these disciplines to achieve the desired impact. Increasing research staff is an option, but it may also be necessary to realign research disciplines within the Department through cross-appointments within IMS or external institutions to achieve a more cohesive thematic platform with well defined missions.