７．点検評価と課題

2017 年度より Hrvoje Petek 教授（ピッツバーグ大学）と中嶋 敦教授（慶應義塾大学）を研究顧問としてお招きし，所全体の研究評価，研究体制についての提言をいただいた。

2021 年 5 月には，米国コロラド大学ボールダー校 Josef Michi 教授より理論・計算分子科学研究領域を中心にヒアリングが実施され，計算科学研究センターの活動も含めてグループの研究内容の評価をいただいた。同じく 2021 年 5 月に，香港科学技術大学 Ching Wan Tang 教授より物質分子科学研究領域を中心にヒアリングが実施され，極端紫外光研究施設（UVSOR）を含めてグループの研究内容及び将来計画の評価をいただいた。

2021 年 10 月に開催された運営顧問会議では，次期中期計画に向けての活動方針（次期所長への申し送り事項）を確認いただいた。

（川合眞紀）

7-1　運営顧問による点検評価

第３期中期計画期間の分子科学研究所活動状況の上で，運営顧問から第４期中期計画期間での運営方針のためのアドバイスをいただくことを目的として，４名の運営顧問を招いて運営顧問会議を開催した。

分子科学研究所の第３期中期計画期間の活動については，2019 年 12 月から 2021 年 7 月にかけて機関の点検・評価が行われた。その結果については，分子研リポート 2019 において，7-1 国際諮問委員会による点検評価，また分子研リポート 2020 において，7-1 大学共同利用機関の教育研究等の検証，7-2 国際諮問委員会の答申リポートとして公開されている。これらを踏まえ，分子科学研究所の抱える課題とそれらへの対応状況を，川合所長から運営顧問に説明した。会議当日には，第４期中期計画期間での研究所機能強化に向けた機関運営方針の提案・検討事項について運営顧問から意見をいただき，分子研側出席者を交えて議論した。会議は所内公開で行い，当日陪席者は 26 名（出席・陪席者総計 45 名）であった。議論された内容は，川合所長より渡辺芳人次期所長に申し送られた。

１．日　時：　2021 年 10 月 21 日（木）10:00 ～ 12:00
２．方　式：　オンライン開催（zoom 会議）
３．出席者：

運営顧問

菊池 昇	（株式会社コンポン研究所 代表取締役所長）
長我部 信行	（株式会社日立製作所 ライフ事業統括本部 CSO）
瀧川 仁	（高エネルギー加速器研究機構 物質構造科学研究所 協力研究員）
松本 吉泰	（公益財団法人豊田理化学研究所 フェロー）

分子科学研究所

川合 眞紀 所長	
岡本 裕巳 教授	（研究総主幹，メゾスコピック計測研究センター長）
斉藤 真司 教授	（理論・計算分子科学研究領域主幹）
大森 賢治 教授	（光分子科学研究領域主幹）
横山 利彦 教授	（物質分子科学研究領域主幹，機器センター長）
飯野 亮太 教授	（生命・錯体分子科学研究領域主幹）
江原 正博 教授	（計算科学研究センター長）
解良 聡 教授	（極端紫外光研究施設長）
山本 浩史 教授	（装置開発室長）
秋山 修志 教授	（協奏分子システム研究センター長）
石﨑 章仁 教授	（理論・計算分子科学研究領域）
繁政 英治 技術推進部長	
中村 敏和 チームリーダー	（機器センター）
福井 豊 URA	（研究力強化戦略室）
亀高 愛 URA	（研究力強化戦略室）

４．議論内容：

国際諮問委員会（2019 年 12 月）での指摘課題

１．極端紫外光研究施設の中長期計画

２．研究領域の再編

３．外国籍研究者の積極的雇用

４．研究所運営業務と教育・研究業務の分離

その他．自己検証での 7 つの指標

現所長からの提案（内容詳細については，参考資料として第 9 章に添付する）

目標 1) 研究所の Visibility の向上

目標 2) 研究所運営業務の効率化

目標 3) 社会との共生

7-2　理論・計算分子科学研究領域の評価

7-2-1　Josef Michl 外国人運営顧問

Report of external review of the Department of Theoretical and Computational Molecular Science at the Institute for Molecular Science, National Institutes of Natural Sciences, Okazaki, Japan

by

Josef Michl, Segur Endowed Chair, Department of Chemistry, University of Colorado Boulder, CO 80309-0215, U.S.A.

May 29, 2021

Overview

Professor Shinji Saito invited me to perform an evaluation of research at the Department of Theoretical and Computational Molecular Science at the Institute for Molecular Science. Because of the Covid-19 pandemic, this was done on-line in the evenings of 17–20 May, 2021 (Mountain Standard Time). I was familiar with the high level of science at the IMS from my previous visits and felt honored to be asked to serve as a Foreign Councilor.

I had very high expectations of scientific quality beforehand and was impressed to find that they were actually exceeded once the review started. I enjoyed an excellent introduction by the director, Professor Maki Kawai, and then a series of uniformly first-class presentations characterized by clarity and enthusiasm. I will provide additional comments on those below. My overall conclusion from the visit is that under the highly competent leadership of Professor Saito, the level of scientific work and accomplishment in the Department is competitive with what is found in the best institutions anywhere in the world. The subjects under investigation are at the frontier of modern condensed phase molecular science and include both advanced nanoscale materials and complex biomolecular systems, encompassing both the latest electronic structure theory at the correlated electron level and powerful molecular dynamics. The work is at the cutting edge of the discipline and has a good balance of method development and highly relevant applications. I found strong collaborative connections to experiments, both within the IMS and nation-wide. The very successful computer center, directed by Professor Ehara, has state-of-theart facilities and represents the focal point of an additional very essential nation-wide network. Importantly, the Department is also strongly networked with global science.

It was heart warming to see that the historic gender imbalance has now started to be addressed. It was also very satisfying to see how many young scientists educated in the Department have been able to secure good appointments elsewhere. The Department is clearly very successful not only in performing world-class theoretical work in molecular science and integrating theory with experiment, but also in its important role of nurturing young talent. This is particularly significant in view of the apparent gradually developing nation-wide shortage of gifted young people interested in a career in theoretical molecular science. It would be beneficial if the supply of first-class domestic and international graduate students at the IMS could be increased and the individual research groups enlarged. Perhaps this could be promoted by setting up prestigious fellowships named for famous Japanese theoreticians, especially those whose names are associated with the IMS, such as Keiji Morokuma. I also wonder whether it would be possible to engage the JSPS in a common international endeavor to attract an increased number of outstanding graduate students. This might compensate to some degree for the handicap of not educating undergraduate students at the IMS itself and therefore not having a natural stream of talent for the graduate school.

The only regrettable aspect of my experience was that the Covid pandemic made it impossible for me to be physically present and to enjoy face-to-face contacts and the traditional Japanese hospitality and culture in person.

Individual research faculty members

Professor Shinji Saito:

The work in this group is first-class and addresses new challenges at the frontier of molecular dynamics. I found the results obtained for the role of fluctuations in excitation energy transfer in the photosynthetic center particularly interesting and the results for water at a wide range of temperatures especially intriguing.

Professor Masahiro Ehara:

The work of this group is characterized by absolutely fearless application of advanced electronic structure methods to most complicated problems, both in photochemistry and photophysics, and in catalysis by metallic nanoclusters, something that very few groups in the world would dare tackle at this level of accuracy. Perhaps because of my own research interests, I was particularly intrigued by the highly original work on inverse design of chiral and other photophysical functional molecular systems. The nation-wide importance of the IMS computer facility operated by Professor Ehara has already been mentioned above.

Professor Akihito Ishizaki:

This research group works at the cutting edge of quantum dynamics in molecules and materials. Its exploration of decoherence and particularly its work on charge separation in photovoltaic devices provided deep insight. The exploration of the combination of quantum optics with molecular photophysics and quantum chemistry is a unique strength and I will be eagerly awaiting further advances in the use of entangled photons in molecular spectroscopy.

Associate Professor Emi Minamitani:

Electron–phonon interactions, with applications ranging from superconductivity, with particular attention to two-dimensional materials, to thermoelectricity, with clever use of neural networks, are the specialty of this high-level research group. Its focus lies deep in solid state physics, with which I unfortunately have too little first-hand experience to be able to make additional comments.

Associate Professor Kei-ichi Okazaki:

The focus of this group is the dynamics of biomolecular machinery operating in living cells and is done in collaboration with experimentalists. This work is at the frontier of what is possible in molecular dynamics since it requires dealing with rare events in very large proteins, using coarse-grained simulations. It addresses the remodeling of membranes and the intriguing issue of unidirectional motion. I find the application to the design of biosensors especially outstanding.

Associate Professor Hisashi Okumura:

This high-quality group performs demanding molecular dynamics simulations of the misfolding and aggregation of proteins responsible for human diseases such as Alzheimer's and Parkinson's, and their possible segregation by ultrasound or infrared laser radiation. It benefits from collaboration with experimentalists both within the IMS and outside. The excellent computational results have allowed it to propose detailed mechanisms and make predictions that were subsequently verified by experiments.

Josef Michl
Segur Chair Professor of Chemistry
University of Colorado at Boulder
Boulder, Colorado 80309-0215
USA

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

June 16, 2021

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.