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

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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.

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