7-3 協奏分子システム研究センターの評価 7-3-1 David A. Leigh 外国人運営顧問 Prof. Dr. Yoshihito Watanabe Director General

Institute for Molecular Science Okazaki Japan

14th December 2023

Dear Director Watanabe,

Evaluation of Various Groups of the NINS Institute for Molecular Science, Okazaki, Japan

Many thanks for the warm and kind hospitality of you and your colleagues during my on-site visit to the NINS Institute for Molecular Science on 3–8 December 2023. During my visit I discussed with you the response to my previous Report (April 2023) and was given in-depth presentations by Prof. Shuji Akiyama, Director of CIMoS, and other members of CIMoS and other parts of IMS. I also attended an excellent interdisciplinary workshop on molecular machines with leading researchers from all over Japan (and online from Strasbourg), organized by Prof. Iino.

1. Response to my Previous (April 2023) Report

I note the significant steps you have taken in response to the recommendations of my April 2023 report. These include:

 To address the relatively small size of IMS groups compared to international competitors you are (i) allowing PIs to hire (through funding from their own grants) associate and/or junior associate professors for research; and (ii) the SOKENDAI (graduate school) is being reorganised which you hope will make it more attractive to PhD applicants.

I hope that these measures prove successful. I believe that the best way to get access to potential graduate schools is to foster closer relationships with universities, as I outlined in my previous Report. But I accept there are practical, and perhaps institutional, reasons why this may be difficult to achieve.

2. To address the substantial gender imbalance amongst PIs I was delighted to learn that you are making three cross-appointment positions at Associate/Full Professor level and that two of these have already been agreed upon. That is a fantastic response and I'm sure will provide role models that will demonstrate to female PhDs and postdocs that a career for them is possible in academic research. I hope that in time that you might also reconsider the removal of the 'no internal promotion' rule for female scientists, in recognition of the unique burden of women in bearing children, as recommended in my previous report. I'm aware that female PhD students and postdocs have mentioned the importance of stability during their late-20s and 30s, when they would (or could) be starting and raising young families. Knowing that they would have to change institution to be promoted is a reason they may not seek a position at IMS.

- 3. I was also delighted to hear that you intend to offer a PI position to a foreign colleague to establish a satellite lab at IMS. This is a great initiative to bring cultural diversity in the way of thinking at PI level to IMS. I think it will be great for Japanese science generally. I am sure that leading scientists in Europe and the US will follow this development closely!
- 4. The cross-appointment with the University of Tokyo of Prof. Makoto Fujita, one of the world's leading scientists, is certainly a boost for the international recognition of IMS.
- 5. I was also impressed with the new multidisciplinary projects you are proposing to bring strengths from different parts of IMS (and elsewhere) together to tackle major scientific problems: Spin-Bioscience—which ranges from the development of novel molecular probes for MRI to magnetic resonance imaging on living organisms— and a project that seeks to leverage IMS's great strengths in photonics and bioscience.

2. Overall impressions

My overall impression of IMS in two visits has been over-whelmingly positive: It is an influential and highly respected institute in the field of the molecular sciences. It is globally renowned for carrying out high quality innovative research, its strong faculty, an excellent research environment, and collaborations with other institutions and universities, all of which make it a leading centre for research internationally. The Institute and Department strengths include that the staff are well motivated and perform at the highest level. The leadership is outstanding. The level of equipment and instrumentation is well above that of many world class laboratories in the USA and Europe. This gives the groups at IMS a significant advantage over competitors worldwide in terms of their ability to tackle the toughest problems in science today. I will not repeat here the other observations discussed in my previous Report.

3. Evaluation of Various Individual Groups of the NINS Institute for Molecular Science

On this visit I had research presentations from 3 members of CIMoS and 2 from other parts of IMS. Two were primarily associated with studies on the molecular basis and mechanisms of biological systems (Akiyama, Okazaki), one working on aspects of materials (Yamamoto) and two working on the application of state-of-the-art spectroscopy to molecular problems (Kuramochi, Kumagai). All of these groups are of very high quality; they tackle important fundamental problems in creative ways and publish their findings in the best international journals.

Prof. Shuji AKIYAMA

PProfessor Akiyama's research focuses on the Circadian clock system in cyanobacteria, in particular the atomic-scale origin of slowness of the cycle and its rhythm, structure and diversity. He is a world leader in these areas, seeking answers to deeply fundamental questions from molecular mechanism to how these extraordinary systems evolved. The group is trying to answer profound scientific questions regarding the way that biology works at the molecular level. The breadth of science being undertaken is remarkable for a single research group, as they seek an understanding of (i) the self-sustained 24 hour oscillation of the system, (ii) the temperature compensation observed, and (iii) the synchronization of the clock. Recent highlights include "*Atomic-scale origins of Slowness in the cyanobacterial Circadian clock*," *Science* **349**, 312–316 (2015), "*Regulation mechanisms of the dual ATPase in KaiC*," *Proc.*

Natl. Acad. Sci. USA 119, e2119627119 (2022) and "Elucidation of master allostery essential for Circadian clock oscillation in cyanobacteria," Sci. Adv. 8, eabm8990 (2022).

Prof. Hiroshi YAMAMOTO

Professor Yamamoto is an international leader in the development of electronics based on π -systems in soft matter. In recent years he has exploited the low dimensionality of the π -electrons to generate materials with a range of different characteristics to silicon. The potential applications of this research range from nano-scale devices to superconductivity and quantum computing. Recent highlights include "*Giant spin polarization and a pair of antiparallel spins in a chiral superconductor*," *Nature* **613**, 479–484 (2023) and "*Highly durable spin filter switching based on self-assembled chiral molecular motor*," *Small* **19**, 2302714 (2023).

Assoc. Prof. Hikaru KURAMOCHI

Associate Professor Kuramochi is an exciting, relatively new, appointment (April 2020) who uses ultrafast spectroscopy to study chemical reaction dynamics. This includes ultrafast spectroscopy at the single molecule level, the development of novel light sources, and the use of advanced ultrafast spectroscopy to study ensembles. Recent highlights include "*Rapid-Scan Resonant Two-Dimensional Impulsive Stimulated Raman Spectroscopy of Excited States*," *J. Phys. Chem. A* **127**, 5276–5286 (2023) and "*Environment-Sensitive Fluorescence of Cot-Fused Perylene Bisimide Based on Symmetry-Breaking Charge Separation*," *Photochem. Photobiolo. Sci.* **22**, 2541–2552 (2023).

Assoc. Prof. Kei-ichi OKAZAKI

Associate Professor Okazaki was a Project Associate Professor at IMS from 2016–2020 and since 2020 has been an Associate Professor at the Research Center for Computational Science. Okazaki's group elucidate the dynamics of biomolecular machines through molecular simulations and other theoretical/computational methods. His growing standing in the field is reflected in his recent co-authorship of an opinion piece on protein folding and folds, from experts in the field ["*Opinion: Protein folds vs. protein folding: Differing questions, different challenges,*" *Proc. Natl. Acad. Sci. USA* **120**, e2214423119 (2023)]. Other recent highlights include "*Molecular mechanism on forcible ejection of ATPase inhibitory factor 1 from mitochondrial ATP synthase,*" *Nat. Commun.* **14**, 1682 (2023) and "*Structure and mechanism of oxalate transporter OxlT in an oxalate-degrading bacterium in the gut microbiota,*" *Nat. Commun.* **14**, 1730 (2023).

Assoc. Prof. Takashi KUMAGAI

Associate Professor Kumagai is another recent appointment, arriving at IMS in 2020. His research focuses on advanced nanospectroscopy with time- and spatially-confined light. While he continues to build new instruments in his lab, he has made good use of instruments from his previous post in Berlin. Recent highlights include "*Inelastic Light Scattering in the Vicinity of a Single-Atom Quantum Point Contact in a Plasmonic Picocavity*," *ACS Nano* **17**, 10172 (2023) and "*Nanoscale coherent phonon spectroscopy*," *Sci. Adv.* **8**, eabq5682 (2022).

I hope that this short report and my previous longer one are useful to you and your colleagues in thinking about how to continue to develop IMS. It is a truly fantastic institute with excellent scientists doing world class research. It has been a pleasure to visit and

interact with such inspiring people, from the young researchers to the thoughtful generous leadership. I hope to visit again and to collaborate with some of the groups there. I wish you and your colleagues much continued success!

Best wishes,

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David A. Leigh FRS Royal Society Research Professor & Sir Samuel Hall Chair of Chemistry, University of Manchester, UK 14 December 2023