

2023年 3月 27日  
(Year/Month/Day)

名古屋大学 大学院情報学 研究科長 殿  
To: Dean of Graduate School of Informatics, Nagoya University

## 研究報告書

### RESEARCH REPORT

滞在期間における研究報告書を、添付のとおり提出いたします。  
This is the cover page of my attached research report.

#### A. Cover Page

1. 被招へい研究者 所属・職・氏名 Affiliation (Country / Area), Position, Name of Visitor Boston University, Department of Chemistry, Boston, MA USA, Professor, John STRAUB
2. 受入研究者 所属・職・氏名 Affiliation, Position, Name of Host Nagoya University, Masataka NAGAOKA
3. 滞在中の研究テーマ Research Theme during the Visit Computer simulations of molecular interfaces in biology and materials science
4. 滞在期間 Period of Visit <u>2023年 3月 5日 ~ 2023年 3月 18日</u> From (Year/Month/Day) To (Year/Month/Day)
5. 招へい教員の主な研究テーマ Main Research Themes of the Visitor Theoretical chemistry; molecular simulations; enhanced sampling algorithms; molecular self-assembly in micelles and membranes; amyloid protein aggregation
6. 招へい教員の個人ページなどへのリンク Link (URL) to the Personal (or Project) Page of the Visitor <a href="https://www.bu.edu/chemistry/profile/john-e-straub/">https://www.bu.edu/chemistry/profile/john-e-straub/</a>

(注) 「研究報告書」には、被招へい研究者の研究活動や講義等の写真を添付してください。なお、「研究報告書」(セクションA, B, C)及び写真は Web サイト等で公開される場合があります。個々の写真の公開を拒否される場合は、その旨記載して下さい。  
Please select pictures which were taken when the visitor conducted his/her research or provided a lecture, and attach it to in this report. We may later upload the reports (sections A, B, and C) and/or pictures on our Web site. If the visitor does not want to have the picture(s) posted on our Web site, please indicate so per picture.

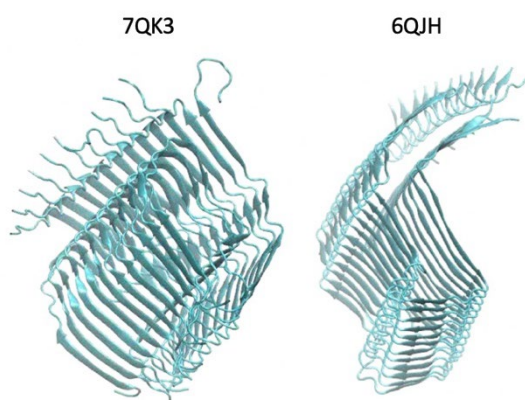
## B. Research Activities (to be published at the Faculty Web Site)

### 1. 滞在中の共同研究テーマや(可能なら)成果の紹介

#### Brief Introduction of the Joint Research and Result (if possible) during the Visit

Molecular interfaces play important roles in biology and in materials science. Examples include membranes and organelles in biology, and electrochemical interfaces in battery science. The simulation of complex molecular interfaces, using chemically accurate models providing atomic-level resolution, remains a substantial challenge.

The Visitor has expertise in the use of enhanced sampling methods for the study of interfaces in biology, including membranes and amyloid formation. Laboratories at Nagoya University have expertise in modeling interfaces (Nagaoka Lab, Nagoya University, Graduate School of Informatics) and solvation (Yoshida Lab, Nagoya University, Graduate School of Informatics). The Visitor also enjoyed research discussions with Professor Ana-Nicoleta Bondar (University of Bucharest) regarding water networks at protein-solvent interfaces. The research discussions during the visit focused on sharing methods and applications related to interfacial science. While no final results can be reported from the research discussions at this time, a number of lines of study were defined for which research has been initiated.



(1) The analysis of water networks surrounding amyloid fibrils (with Professor Ana-Nicoleta Bondar): Certain amyloid-forming proteins are known to form fibrils with multiple structures – known as polymorphs. The prediction of polymorphic structures, and developing an understanding of the origins of polymorphism, represent outstanding research goals in the amyloid field. Past work on amyloid fibril formation by the Visitor identified an important role for water networks within the fibril in directing the formation of one polymorphic structure or another.

The Visitor learned of the work of Professor Bondar on identifying water networks for given protein structures. The Visitor plans to share structural models of various polymorphic fibrils, developed in the Visitor's lab, or analysis by Professor Bondar.

(2) The analysis of solvation of amyloid fibrils using 3D-RISM (with Professor Norio Yoshida): The Visitor has an interest in understanding the role of solvation in protein liquid-liquid phase separation, particularly in the context of amyloid formation. The Visitor discussed the possible application of 3D-RISM methods with Professor Yoshida, which will serve as a complement to the all-atom solvation models currently used in the Visitor's lab.

(3) Finally, the possible organization of a future research workshop on theoretical methods for study the role of solvation and interfaces, including scientists from Japan, Europe, and North America (with Professor Masataka Nagaoka and Professor Norio Yoshida).

### 2. 滞在中に訪問した研究者

#### Researcher(s) Visited during the Stay

The Visitor also enjoyed discussions on the campus of Nagoya University. Researchers included Professor Masataka Nagaoka (Nagoya University, Graduate School of Informatics) and Professor Norio Yoshida (Nagoya University, Graduate School of Informatics).

Additional discussions were held with Nagoya University faculty, including Professor Yuko Okamoto (Nagoya University, Computer Center); and Professor Takahisa Yamato (Nagoya University, Graduate School of Physics); Professor Hedong Zhang (Nagoya University, Graduate School of Informatics), Dr. Yuichi Tanaka (Nagoya University, Graduate School of Informatics) and Mr. Yuki Shirasawa (Nagoya University, Graduate School of Informatics).

In addition, the Visitor enjoyed discussions with Professor Tetsuro Nagai (Fukuoka University); Professor Ana-Nicoleta Bondar (University of Bucharest). Additional scientific discussions included brief exchanges with Professor Florence Tama (Nagoya University, Graduate School of Physics), Dr. Osamu Miyashita (RIKEN Center for Computational Science), and Professor Fumio Hirata (retired).

### 3. 滞在中に参加したワークショップなど

#### Workshop/Symposium/Conference Attended during the Visit

The Visitor enjoyed lectures and interactions during a two-day Study Camp held at Ohmi-Hachiman (6-7 March 2023). The program was rich in presentations students from the Nagaoka Laboratory, including a postdoctoral researcher (Tanaka), doctoral student (Kanesato), and masters students (Kondo, Fujita, Inagaki, Shirasawa, and Yotsuya).

In addition, there were presentations from senior researchers including the Visitor, and Professors Bondar (University of Bucharest), Ehara (Institute for Molecular Science), Otani (University of Tsukuba), Matubayasi (Osaka University), Yoshida (Nagoya University), Kasahara (Osaka University), Kitamura (Shizuoka University), Kayanuma (National Institute of Advanced Industrial Science and Technology), and Okita (Osaka University). The scientific presentations were of great interest to the Visitor and the scientific discussions were many and excellent.



In addition, Professor Nagaoka organized and hosted a Future Value Creation Research Center (FV-CRC) Symposium (15 March 2023) with presentations by the Visitor and Professor Ana-Nicoleta Bondar (University of Bucharest). The symposium was well attended by Nagoya University faculty and students, as well as visiting scientists Professor Fumio Hirata (retired) and Professor Tetsuro Nagai (Fukuoka University). The discussions following each talk were highly engaging and led to a number of continuing discussions with the Visitor that have been of great value.





## C. Life in Nagoya/Life in Japan (to be published at the Faculty Web Site)

観光/食/文化などなんでも。

名古屋あるいは日本に滞在して楽しかったことや印象に残ったことなど。

(Sightseeing, Food, Culture, etc. Please describe whatever you felt interesting or impressive during your stay in Nagoya and Japan.)

The Visitor has enjoyed many trips to Japan since the late 1990s. This visit was particularly special as it was the Visitor's first return to Japan since 2019, due to the recent pandemic. In addition, the scientific interactions and cultural excursions were interesting and enjoyable. I am especially grateful to Professor Nagaoka for his exceptional work in organizing our activities and generously serving as our guide.



The Visitor enjoyed participating in the science and cultural events associated with a two-day Study Camp organized by Professor Nagaoka. We stayed on the shore of Lake Biwa and also had a half-day cultural excursion to Ohmi-Hachiman.

We began with delicious “Japanese home cooking” at a local restaurant, which had a wonderful atmosphere. In addition, we enjoyed a ride on the ropeway to the top of Mount Hachiman and had a hiking excursion to explore the Hachiman castle ruins. We also enjoyed an interesting boat trip on the canals of the town. We learned the importance of the canal in earlier times, for the transport of goods to Kyoto and Osaka. The quaint scenery made us feel we had returned to earlier times in Japan. Finally, we had a walk about town that included a visit to Himure-Hachimangu Shrine which was very beautiful.

In Nagoya, the Visitor enjoyed many wonderful meals. No visit to Nagoya is complete without a delicious Hitsumabushi lunch at Atsuta Hitsumabushi. The Visitor also enjoyed being treated to a meal of Nagoya-style chicken wings at a local restaurant in Motoyama, with many faculty in attendance. This was a kind gesture and made for an enjoyable evening. Finally, I returned to Maruhachi Sushi in Yagoto with Professors Masataka Nagaoka and Yuko Okamoto.