# Shun Yokoi, Ph.D.

## Personal Information

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## Education

**Ph.D. in Science (GPA: 4.0/4.0)** **April 1st 2022—March 26th 2025**
Department of Physics, Graduate School of Science and Technology, Meiji University, Tokyo, Japan
Dissertation Title: "Computational Insights into the Activation Mechanism of Orexin 2 Receptor from Extensive Molecular Dynamics Simulations and Relaxation Mode Analysis"
Advisor: Ayori Mitsutake, Ph.D., Meiji University

**M.A. in Science (GPA: 4.0/4.0)** **April 1st 2020—March 26th 2022**
Department of Physics, Graduate School of Science and Technology, Meiji University, Tokyo, Japan
Coursework: Biophysics, Computational Physics/Chemistry, Machine Learning, Deep Learning, etc.

**B.A. in Science** **April 1st 2016—March 26th 2020**
Department of Physics, School of Science and Technology, Meiji University, Tokyo, Japan
Coursework: Quantum Mechanics, Electromagnetic, Statistical Mechanics, Optics, Physical Mathematics, Biophysics, Information Processing, etc.

## Research Experience

**Researcher** **April 2025—Present**
International Institute for Integrative Sleep Medicine (WPI-IIIS), University of Tsukuba
- Conducting drug design research involving protein complex structure modeling, docking calculations, extensive molecular dynamics simulations, data analysis, etc.

**Research Fellow for Young Scientists** **April 2023—March 2025**
Japan Society for the Promotion of Science (JSPS)
- Leading a research project titled "Proposal of G Protein-biased Agonist for Orexin 2 Receptor based on Computational Chemistry and Physics".

**Visiting Scholar** **March 2022—July 2023**
Biological Sciences Division, SLAC National Accelerator Laboratory / Department of Structural Biology, School of Medicine, Stanford University (Supervisor: Soichi Wakatsuki, Ph.D.)
- Collaborate with experimental groups to clarify the function and dynamics of mitochondrial fission 1 protein, ribosomal 30S subunit, and the SARS-CoV-2 papain-like protease using integrated experimental and computational approaches.
- Learning laboratory techniques such as protein expression, purification and structural analysis (X-ray crystallography, Cryo-EM), etc.

**Research Associate** **April 2022—March 2023**
School of Science and Technology, Meiji University (Supervisor: Ayori Mitsutake, Ph.D.)
- Performed simulations and developed analysis methods to investigate activation and biased-signaling mechanisms of G protein-coupled receptors (GPCRs).

## Honors and Awards

- Matsuo Research Award, The GPCR Meeting of Japan **May 2024**
- Student Prize, The Molecular Simulation Society of Japan **December 2023**
- Excellent Presentation Award, The Chem-Bio Informatics Society of Japan **October 2023**
- Taylor & Francis Molecular Simulation Prize, International Union of Pure and Applied Physics (IUPAP) **August 2023**
- JSPS Research Fellowship for Young Scientists, Japan Society for the Promotion of Science **April 2023**
- The 13th Meiji University Graduate School Dean's Award, Meiji University **March 2022**
- The 14th TOBITATE! Young Ambassador, Japan's Ministry of Education, Culture, Sports, Science, and Technology (MEXT) **July 2021**
- Student Presentation Award, The Biophysical Society of Japan **September 2020**

## Grants and Scholarship

- International Collaborative Research Promotion Project, Meiji University **July 2024**
- JSPS Research Fellowship for Young Scientists, Japan Society for the Promotion of Science **April 2023**
- Researcher New-mode Mobility Accelerator Program, Japan Science and Technology Agency **February 2023**
- Meiji University Graduate Research Scholarship A, Meiji University **April 2023**

- Natural sciences/cross-disciplinary course, The 14th TOBITATE! Young Ambassador Program, Japan Public-Private Partnership Student Study Abroad Program, Japan's Ministry of Education, Culture, Sports, Science, and Technology (MEXT) **July 2021**

## Publications

- **Yokoi S**, Mitsutake A, "Investigation of GPCR dynamics using large-scale molecular simulations", *The Cell*, 57(3), 51-53 (2025). [In Japanese]
- **Yokoi S**, Suno R, Mitsutake A, "Structural and Computational Insights into Dynamics and Intermediate States of Orexin 2 Receptor Signaling", *J Phys Chem B,* 128, 6082-6096 (2024). [Featured as a journal front cover of *The Journal of Physical Chemistry B*]
- Suno-Ikeda C, Nishikawa R, Suzuki R, **Yokoi S** *et al*, "Structural and Dynamic Insights into the Biased Signaling Mechanism of the Human Kappa Opioid Receptor" (*in revision*, *Nature Communications*)
- Yapici I, Dao E H, **Yokoi S** *et al,* "Unlocking Protein-RNA Interactions: Time-Resolved Serial Crystallography of Ribosome-IF1 as a Paradigm" (*under review, The EMBO Journal*).
- Pokhrel S, Heo G, Mathews I, **Yokoi S** *et al*, "A hidden cysteine in Fis1 targeted to prevent pathological mitochondrial fission and dysfunction" (*review complete*, *Nature Communications*)
- **Yokoi S**, "Structural and Computational Insight into Dynamics and Intermediate State in Activation of Orexin 2 Receptor", *Ensemble*, 26, 115-116 (2024). [In Japanese]
- Yapici I, Dao E H, **Yokoi S** *et al,* "4D Crystallography Captures Transient IF1-Ribosome Dynamics in Translation Initiation", *bioRxiv*, doi: 10.1101/2023.10.27.564398.
- **Yokoi S**, "Overseas Introduction: My stay at Stanford University in the U.S. - What I learned and felt at Stanford University", *Ensemble*, 25, 243-250 (2023). [In Japanese]
- **Yokoi S**, Mitsutake A, "Characteristic Structural Difference between Inactive and Active States of Orexin 2 Receptor Determined Using Molecular Dynamics Simulations", *Biophys Rev,* 14, 221-231 (2022).
- **Yokoi S**, Mitsutake A, "Molecular Dynamics Simulations for Determination of the Characteristic Structural Differences between Inactive and Active States of Wild-type and Mutants of the Orexin2 Receptor", *J Phys Chem B,* 125, 4286–4298 (2021). [Featured as a supplementary cover of *The Journal of Physical Chemistry B*]

## University Service

**Teaching Assistant** **April 2023—March 2024**
School of Science and Technology, Meiji University
Courses: Physical Mathematics, Electromagnetism

**Research Assistant** **July 2021—February 2022**
Research and Intellectual Property Strategy Organization, Meiji University

**Teaching Assistant** **April 2021—February 2022**
Learning Support Office, School of Science and Technology, Meiji University

**Teaching Assistant** **April 2021—February 2022**
School of Science and Technology, Meiji University
Courses: Physical Mathematics, Laboratory Experiments on Physics

**Research Assistant** **December 2020—March 2021**
Graduate School of Science and Technology, Meiji University

**Research Supporter** **April 2019—March 2020**
Center for Gender Equality and Diversity, Meiji University

## Work Experience

**Tutor (Private Individual Tuition)** **April 2016—February 2022**
TOMAS, Riso Kyoiku
Taught mathematics and science to elementary through high school students, with 40+ students accepted into their desired schools.

## Internship Experience

**Bootcamp for Digital Transformation (DX) Professionals** **August 2023—September 2023**
AGC Inc., Acaric Co., Ltd., and Mamezou Co., Ltd.
- Acquired data analysis fundamentals through coursework, case studies, and Python-based hands-on training.
- Built and proposed a machine learning–based defective product detection model.

## Volunteer Work

- Boat Crew of a Signal Boat, Tokyo 2020 Summer Olympics **June 2021—August 2021**
- Boat Crew of a Signal Boat, READY STEADY TOKYO **August 2019**
- Boat Crew of a Mark Boat, World Cup Series: Enoshima **September 2018**

## Conference Presentations

- "Computational Insights into Dynamics and Intermediate States of Orexin 2 Receptor Signaling", The Sugadaira Winter Workshop 2025 on the role of fluctuations and dynamics in bio and soft matter, January 2025
- "Structural and Computational Insights into Dynamics and Intermediate States of Orexin 2 Receptor Signaling", Stanford Bio-X Interdisciplinary Initiatives Seed Grants Program Symposium and Poster Session, August 2024
- "Structural and Computational Insights into Dynamics of Biomolecules using Molecular Dynamics Simulations", International Institute for Integrative Sleep Medicine (WPI-IIIS) Special Student Seminar, July 2024
- "Complementary Analysis between 4D Crystallography and Extensive MD Simulation Captures Transient IF1-Ribosome Dynamics in Translation Initiation", The 21st IUPAB & 62nd BSJ Joint Congress 2024, June 2024
- "Structural and Computational Insights into Dynamics and Intermediate States of Orexin 2 Receptor Signaling", The 24th Annual Meeting of the Protein Science Society of Japan, June 2024
- "Structural and Computational Insights into Dynamics and Intermediate States of Orexin 2 Receptor Signaling", The 18th GPCR meeting, May 2024
- "Structural and Computational Insights into Dynamics and Intermediate States of Orexin 2 Receptor Signaling", Gordon Research Conference –Ligand Recognition and Molecular Gating–, March 2024
- "Structural and Computational Insight into Dynamics and Intermediate State in Activation of Orexin 2 Receptor", The 11th Young Scientists' Seminar in Chem-Bio Informatics Society, March 2024
- "Investigation of the Structures and Dynamics of Biomolecules using Molecular Dynamics Simulations", Student Seminar at Boston University, March 2024
- "Computational Insights into Activation Mechanism of Orexin 2 Receptor using Large-scale Molecular Dynamics Simulations", The 37th Symposium of the Molecular Simulation Society of Japan, December 2023
- "Structural and Computational Insight into Dynamics and Intermediate States of Orexin 2 Receptor Activation", "Molecular Movies" International Symposium 2023, November 2023
- "Structural and Computational Insight into Dynamics and Intermediate State in OX2R Activation", The 61st Annual Meeting of the Biophysical Society of Japan, November 2023
- "Structural and Computational Insight into Dynamics and Intermediate States in Orexin 2 Receptor Activation", The 5th "Molecular Movies" Young Scientists Online Seminar, November 2023
- "Structural and Computational Insight into Dynamics and Intermediate State in Activation of Orexin 2 Receptor", Chem-Bio Informatics Society Annual Meeting 2023, October 2023
- "Structural and Computational Insight into Dynamics and Intermediate State in Activation of Orexin 2 Receptor", The 5th conference of Theory and Applications of Computational Chemistry (TACC), September 2023
- "Computational Insight into Dynamics and Intermediate State in OX2R Activation", 34th IUPAP Conference on Computational Physics (CCP2023), August 2023
- "The Value of Studying Abroad for Undergraduate and Graduate Students", Building networks of diverse and highly talented researchers, Japan-U.S. Research Collaboration Week, July 2023
- "Study for Structure and Dynamics Using Computer Simulation", The 5th Japanese Academic Seminars at Stanford, December 2022
- "Computational insights into the dynamics and intermediate states of OX2R activation", The 36th Symposium of the Molecular Simulation Society of Japan, December 2022
- "Computational Insight into Dynamics and Intermediate States in OX2R Activation based on Molecular Dynamics Simulations", Stanford Bio-X Interdisciplinary Initiatives Seed Grants Program Symposium and Poster Session, August 2022
- "Dynamics of the Complex for Orexin 2 Receptor and G protein using Molecular Dynamics Simulations", The 36th Anniversary Symposium of The Protein Society, July 2022
- "Structural Dynamics Research for Wild-type and Mutants of Orexin 2 Receptor using Computational Modeling and Molecular Dynamics Simulations", The 2nd Transatlantic ECI GPCR Symposium, July 2022
- "Molecular Dynamics Simulations for Determination of the Characteristic Structural Differences between Inactive and Active States of Wild-type and Mutants of the Orexin 2 Receptor", Molecular Movies International Symposium 2022, May 2022
- "Dynamics of Orexin 2 Receptor and G protein Complex with Molecular Dynamics Simulations", The 35th Symposium of the Molecular Simulation Society of Japan, December 2021
- "Dynamics of Orexin 2 Receptor and G-protein Complex with Molecular Dynamics Simulations", The 59th Annual Meeting of the Biophysical Society of Japan, November 2021
- "Dynamics of Orexin 2 Receptor and G protein Complex with Molecular Dynamics Simulations", The 18th GPCR meeting, November 2021
- "Dynamics of Orexin 2 Receptor and G protein Complex with Molecular Dynamics Simulations", Chem-Bio informatics Society (CBI) Annual meeting 2021, October 2021

- "Structural Dynamics of Orexin2 Receptor for Class A GPCRs," The 35th Virtual Anniversary Symposium of the Protein Society, July 2021
- "Structural Dynamics of Orexin2 Receptor Using Molecular Dynamics Simulations," The 21st Annual Meeting of the Protein Science Society of Japan, June 2021
- "Dynamics of the Orexin 2 Receptor for Class A GPCRs.," The 1st workshop on biomolecular simulations and modeling, March 2021
- "Structural Dynamics of Orexin 2 Receptor Using Molecular Dynamics Simulation," The 76th Annual Meeting of the Physical Society of Japan, March 2021
- "Dynamics of Orexin 2 Receptor Using Molecular Dynamics Simulation," The 34th Symposium of the Molecular Simulation Society of Japan, December 2020
- "Dynamics of Orexin 2 Receptor Using Molecular Dynamics Simulation," The 58th Annual Meeting of the Biophysical Society of Japan, September 2020
- "Dynamics of Orexin Receptors Using Molecular Dynamics Simulations," The 20th Annual Meeting of the Protein Science Society of Japan, July 2020

## Skills and Qualifications

- Molecular Dynamics, Computational Chemistry Methods, and Data Analysis
  - AMBER and GROMACS MD software, CHARMM-GUI, VMD, Chimera, PyMOL, Modeller, AlphaFold2, MOE, Maestro, Gaussian 16, Biopython, Autodock, etc.
- Python, C language, FORTRAN, Microsoft Office (Word, Excel, PowerPoint), Adobe (Acrobat, Photoshop, Premier Pro, Illustrator)
- Driver's license both in Japan and in the U.S., Small vessel operator license, Calligraphy teacher's license

## Language Skills

- Japanese – Native
- English – Proficient

  Study at TALK English School in Atlanta, Georgia USA in August 2017.
  Research at SLAC National Accelerator Laboratory and Stanford University from March 2022 to July 2023.

## Professional Memberships

・The Biophysical Society of Japan ・The Molecular Simulation Society of Japan
・Protein Science Society of Japan ・The Physical Society of Japan ・The Chem-Bio Informatics Society

## Additional Activities

**Meiji University Sailing Team** **April 2016—March 2020**

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| Major results in 2019: | Kanto Student Yachting Individual Championships | 3rd |
| | 470 Class Japan Championships | 5th |
| | All Japan Intercollegiate Yacht Championships in 470 Class | 5th |
| | All Japan Intercollegiate Yacht Championships | 6th |

## Interests and Hobbies

・Sailing ・Soccer ・Traveling