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" (Supervisor: Ayori Mitsutake, Ph.D.)

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, etc.

Research Experience

Visiting Postdoctoral Scholar **July 2025—Present**
Department of Structural Biology, School of Medicine, Stanford University (PI: Soichi Wakatsuki, Ph.D.)
- Integrating computational simulations with experimental approaches to enable protein engineering of next-generation magneto-optogenetic tools, and drive the development of new therapeutic compounds of enzymes.

Postdoctoral Researcher Associate **April 2025—Present**
International Institute for Integrative Sleep Medicine (WPI-IIIS), Tsukuba Institute for Advanced Research (TIAR), University of Tsukuba (PI: Tsuyoshi Saitoh, Ph.D.)
- Conducting drug-design research on G protein–coupled receptors, including protein–complex structure modeling, docking calculations, extensive molecular dynamics simulations, and in-depth computational data analysis.

Visiting Scholar **April 2025—Present**
Organization for the Strategic Coordination of Research and Intellectual Properties, Meiji University
- Developing and applying advanced sampling simulation methods, novel analysis workflows, and generalized relaxation mode analysis.

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

Visiting Student Scholar **March 2022—July 2023**
Biological Sciences Division, SLAC National Accelerator Laboratory (Supervisor: Soichi Wakatsuki, Ph.D.)
- Collaborated with experimental groups to clarify the dynamics of mitochondrial fission protein, ribosomal 30S subunit, and the SARS-CoV-2 papain-like protease using integrated experimental and computational approaches.
- Learned laboratory techniques, such as protein expression, purification, X-ray crystallography, and Cryo-EM.

Research Associate **April 2022—March 2023**
School of Science and Technology, Meiji University (Supervisor: Ayori Mitsutake, Ph.D.)
- Investigated activation mechanisms of orexin 2 receptor using MD simulations and developed analysis methods.

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 **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**
- Student Presentation Award, The Biophysical Society of Japan **September 2020**

Grants, Fellowships, and Scholarships

- Grant-in-Aid for Research Activity Start-up, Japan Society for the Promotion of Science **September 2025**
- RECONNECT Fellows, International International Institute for Integrative Sleep Medicine **July 2025**
- Academic Research Grants (Natural Sciences Division), Mishima Kaiun Memorial Foundation **June 2025**
- IIIS Start-up Grant, International International Institute for Integrative Sleep Medicine **June 2025**
- 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**
- 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

- Johnson JA, Tosun B, …, **Yokoi S**, Wakatsuki S, DeMirci H, "Crystal structure of 3-hydroxypropionyl-CoA synthetase (ADP-forming) from Nitrosopumilus maritimus", *Curr Res Struct Biol*, 11, 100189 (2026).
- Kobayashi K*, Kawakami K*, Matsui T*, **Yokoi S*,** *et al*, "The dynamic basis of G-protein recognition and activation by a GPCR", *Nature*, doi: 10.1038/s41586-026-10228-w (2026). (*co-first authors)
- **Yokoi S**, Mitsutake A, "Computational approaches to understanding G protein-coupled receptor function" (*in revision, Protein Dynamics: Experimental and Computational Approaches*)
- 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", *Nat Commun*, 16, 9392 (2025).
- Ayan E, Engilberge S, **Yokoi S**, *et al*, "Triple Calcium Binding Stoichiometry in the Monoclinic Crystal Form of Protracted Insulin", *Small Structure*, e202500398 (2025).
- Pokhrel S, Heo G, Mathews I, **Yokoi S**, *et al*, "A hidden cysteine in Fis1 targeted to prevent pathological mitochondrial fission and dysfunction", *Nat Commun*, 16, 4187 (2025).
- **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*]
- **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 maths and science to 40+ students in elementary through high school 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

- "Conformational dynamics governing G-protein recognition and activation by Neurotensin Receptor 1", 2026 Spring Bay Area CryoEM Meeting, April 2026
- "Development of Collaborative Networks for Complementary Data Analysis between Molecular Simulations and Experiments on Biomolecular Systems", European Molecular Biology Laboratory (EMBL) – Stanford Life Science Alliance (LSA) Workshop, SLAC National Accelerator Laboratory, March 2026
- "Structural and Computational Insights into Biomolecular Dynamics and Therapeutic Discovery", JSPS San Francisco Japanese Researcher Gathering, February 2026
- "Exploring Activation Dynamics and Conformational Landscapes of GPCRs using Molecular Dynamics Simulations", GPCR Workshop 2025, December 2025
- "Structural and Computational Insights into Biomolecular Dynamics and Therapeutic Discovery", Stanford Bio-X Seed Grants Poster Session, August 2025
- "From Japan to Stanford: My Journey through Computational Biophysics and Global Collaboration", Japan–U.S. Research Collaboration Week 2025, July 2025
- "Beyond Boundaries: The Future of Life Sciences Driven by Physics and Computation", Meiji Univ., June 2025
- "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

- Virtual Screening with Integrated Physics and Machine Learning, Target Enablement, Preparation, and Validation, Applications of Free Energy Calculations in Modern Drug Hunting, Teaching with Schrödinger Introduction (offered by Schrödinger, Inc.)
- 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 Vina, etc.
- Python, C language, FORTRAN, Microsoft Office, 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, Beginner Barbecue Instructor

Language Skills

・Japanese – Native ・English – Proficient ・Spanish – Beginner

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**

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