WPI-IIIS Seminar

Special Student Seminar

Structural and Computational Insights into Dynamics of Biomolecules using Molecular Dynamics Simulations

Molecular dynamics (MD) simulation is a powerful method to investigate the atomic-level dynamics of biomolecules related to functions which cannot be easily obtained from static structural data. Improving computational methods, developing dynamics analysis methods, and increasing computational power has made it possible to perform large-scale and long-term calculations, thus filling the gap between experimental and computational approaches. Recently, I have investigated the dynamics of orexin 2 receptor using extensive MD simulations and conducted research on the mitochondrial fission 1 protein and small 30S ribosomal subunit in an integrated collaboration with experimental and computational approaches. In the seminar, I will present about these recent studies and outlook for future research.

Mr. Shun Yokoi

Ph.D. Candidate

Department of Physics, School of Science and Technology, Meiji University

Date: **Tuesday, July 9, 2024**

Time: **11:00 – 12:00**

Venue: **1F Auditorium, IIIS Building**

✻On-site participation only

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