CURRICULUM VITAE

Shijie Xu

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Date of Birth

March 9th, 1995

Education

Ph.D. in Environmental Science, Hokkaido University

M.Sc. in Computer Science, University of Science and Technology of China

B.Sc. in Mathematics, University of Science and Technology of China

March 2025 (expected) June 2020 June 2017

Research Interests

Bioinformatics, Deep Learning, Computational Chemistry, Computer Science, Mathematics

Skills

Programming: Python / PyTorch / C++ / LATEX/ Bash / Fortran / Rust / HTML / Javascript / Flask /

Django / Go / Coq / Mathematica / MATLAB / Haskell

Softwares: AutoDock Vina / PyMOL / GIMP / Powerpoint / Git / Docker / VSCode **Hardware:** GPU workstation building / Linux server maintenance / Raspberry Pi

Languages: English (fluent), Chinese (native), Japanese (basic)

Publications

- 1. <u>Shijie Xu</u> and Akira Onoda*. "PsiPartition: Improved Site Partitioning for Genomic Data by Parameterized Sorting Indices and Bayesian Optimization." *Journal of Molecular Evolution* 92: 874-890, **2024**, *DOI*: https://doi.org/10.1007/s00239-024-10215-7
- 2. <u>Shijie Xu</u> and Akira Onoda*. "Accurate and Fast Prediction of Intrinsically Disordered Protein by Multiple Protein Language Models and Ensemble Learning." *Journal of Chemical Information and Modeling* 64(7): 2901-2911, **2023**, *DOI*: https://doi.org/10.1021/acs.jcim.3c01202
- 3. Shijie Xu and Akira Onoda*. "Accurate and Rapid Prediction of Protein pK_a : Protein Language Models Reveal the Sequence- pK_a Relationship." Under review.

Presentations

- <u>Shijie Xu</u> and Akira Onoda, "Accurate and Fast Prediction of Protein p K_a by Protein Language Model," 8th ICReDD International Symposium, 22nd Oct 24th Oct 2024, Sapporo, Japan. [Poster]
- <u>Shijie Xu</u> and Akira Onoda, "Accurate Prediction of Intrinsically Disordered Protein by Protein Language Models," the 24th Annual Meeting of the Protein Science Society of Japan, 11th Jul 13th Jul 2024, Sapporo, Japan. [Poster]
- Shijie Xu and Akira Onoda, "Accurate Prediction of Protein pK_a by Geometric Deep Learning," the 104th CSJ annual meeting, 18th Mar 21st Mar 2024, Funabash, Japan. [Oral]
- <u>Shijie Xu</u> and Akira Onoda, "Accurate Prediction of Intrinsically Disordered Protein by Protein Language Models," the 17th Biorelevant Chemistry Symposium, 8th Sep 10th Sep 2023, Chiba, Japan. [Poster]
- <u>Shijie Xu</u> and Akira Onoda, "Fast and Accurate Prediction of Intrinsically Disordered Protein by Protein Language Model," the 103rd CSJ annual meeting, 22nd Mar 25th Mar 2023, Chiba, Japan. [Oral]

Awards, Fellowships, and Grants

- Program for Supporting Challenging and Interdisciplinary Research Field, 2022, 2023, 2024
- Hokkaido University DX Doctoral Fellowship, 2022-2025
- Outstanding Student Scholarship, University of Science and Technology of China, 2016
- S.-T. Yau College Student Mathematics Contests, Beijing, China, 2016
- Outstanding Freshman Scholarship, University of Science and Technology of China, 2014
- First Prize Winner in National High School Mathematics League, Hefei, Anhui, China, 2012

Rearch Experience

Oct 2021 - Mar 2022, Graduate School of Environmental Science, Hokkaido University, Japan, "Accelerating Biohybrid Catalysis Screen via Machine Learning", supervised by Prof. Akira Onoda