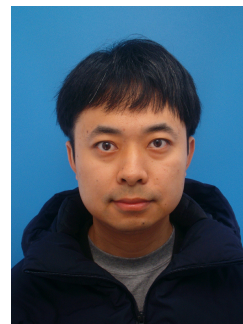


CURRICULUM VITAE

Shijie Xu

Graduate School of Environmental Science, Hokkaido University
Kita-10 Nishi-5, Kita-ku, Sapporo, Hokkaido, 060-0810, Japan

shijie.xu@ees.hokudai.ac.jp • [xu-shi-jie.github.io](https://github.com/xu-shi-jie)



Date of Birth

March 9th, 1995

Education

Ph.D. in Environmental Science, Hokkaido University	March 2025 (expected)
M.Sc. in Computer Science, University of Science and Technology of China	June 2020
B.Sc. in Mathematics, University of Science and Technology of China	June 2017

Research Interests

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

Skills

Programming: Python / PyTorch / C++ / \LaTeX / Bash / Fortran / Rust / HTML / Javascript / Coq / Mathematica / MATLAB / Go / Haskell

Softwares/Tools: AutoDock Vina / PyMOL / GIMP / Powerpoint / Git / Docker / VSCode

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

Publications

1. Shijie Xu 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 DOI: <https://doi.org/10.1021/acs.jcim.3c01202>
2. Shijie Xu and Akira Onoda*. “PsiPartition: Improved Site Partitioning for Genomic Data by Parameterized Sorting Indices and Bayesian Optimization.” Accepted by *Journal of Molecular Evolution*
3. Shijie Xu and Akira Onoda*. “Accurate and Rapid Prediction of Protein pKa: Protein Language Models Reveal the Sequence-pKa Relationship.” Under review.

Presentations

- Shijie Xu and Akira Onoda, “Accurate Prediction of Protein p*K*_a by Geometric Deep Learning,” the 104th CSJ annual meeting, 18th Mar - 21st Mar 2024, Funabashi, Japan. [Oral]
- Shijie Xu 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]
- Shijie Xu and Akira Onoda, “Accurate and Fast Prediction of Protein p*K*_a by Protein Language Model,” 8th ICR₂DD International Symposium, 22nd Oct - 24th Oct 2024, Sapporo, Japan. [Poster]
- Shijie Xu 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 Intrinsically Disordered Protein by Protein Language Models,” the 17th Biorelevant Chemistry Symposium, 8th Sep - 10th Sep 2023, Chiba, Japan. [Poster]

Awards, Fellowships, and Grants

- Program for Supporting Challenging and Interdisciplinary Research Field, 2022, 2023
- 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

Research 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