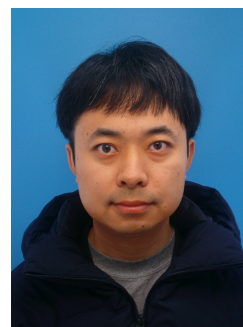


# CURRICULUM VITAE

## Shijie Xu

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### Date of Birth

March 9th, 1995

### Education

Ph.D. in Environmental Science, Hokkaido University	March 2025 (expected)
<i>Dissertation Title:</i> “Accurate and Fast Predictions of Protein Structures and Properties via Protein Language Models”	
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++ /  $\text{\LaTeX}$  / Bash / Fortran / Rust / HTML / Javascript / FastAPI / Flask / Django / Go / Mathematica / MATLAB / Coq / 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. [Shijie Xu](#) 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. [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, **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**

- Shijie Xu and Akira Onoda, “Accurate and Fast Prediction of Protein  $pK_a$  by Protein Language Model,” 8th ICRDD 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 Protein  $pK_a$  by Geometric Deep Learning,” the 104th CSJ annual meeting, 18th Mar - 21st Mar 2024, Funabashi, Japan. [Oral]
- 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]
- 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]

## **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

## **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