CURRICULUM VITAE

Shijie Xu

Faculty of Environmental Earth Science, Hokkaido University
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Date of Birth

March 9th, 1995

Education

Ph.D. in Environmental Science, Hokkaido University	March 2025
Dissertation Title: "Accurate and Fast Predictions of Protein Structures and Properties via Protein Language Models"	
M.S. in Computer Science, University of Science and Technology of China	June 2020
B.S. in Mathematics, University of Science and Technology of China	June 2017

Research Experience

Postdoctoral Researcher, Hokkaido University	April 2025 - Present

Research Interests

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

Skills

Programming: Python / C++ / CUDA / LaTeX/ FORTRAN / Rust / Mathematica / MATLAB / Coq / Haskell
Web development: HTML / JavaScript / FastAPI / Flask / Django / Go
Software: AutoDock Vina / PyMOL / Git / Docker / Singularity / VSCode
Hardware: GPU workstation building / Linux server maintenance / Raspberry Pi
Languages: English (fluent), Japanese (basic), Chinese (native)

Publications

1. Shijie Xu, Ke Xu, and Akira Onoda*. "Accurate Prediction of Enzymatic Degradation of Plastics by Language Models." *Chemistry Letters*, **2026**, *DOI:* https://doi.org/10.1093/chemle/upag022

2. <u>Shijie Xu</u> and Akira Onoda*. "Probe-Based Identification of Metal-Binding Sites Using Deep Learning Representations." *Under Review*, **2025**.

3. <u>Shijie Xu</u> and Akira Onoda*. "Accurate and Rapid Prediction of Protein pK_a: Protein Language Models Reveal the Sequence-pK_a Relationship." *Journal of Chemical Theory and Computation* 21(7): 3752–3764, **2025**, *DOI:* https://doi.org/10.1021/acs.jctc.4c01288

4. <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

5. <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, **2024**, *DOI:* https://doi.org/10.1021/acs.jcim.3c01202

Presentations

- <u>Shijie Xu</u> and Akira Onoda, "Accurate and Fast Prediction of Protein pK_a by A Protein Language Model", the 19th Symposium on Biorelevant Chemistry, 2nd Sep - 4th Sep, 2025, Kyoto, Japan. [Poster]

- <u>Shijie Xu</u> and Akira Onoda, "Accurate and Fast Prediction of Protein pK_a by Protein Language Model", 51st Biomolecule Science Symposium, 26th Oct - 27th Oct 2025, Sapporo, Japan. [Oral]

- <u>Shijie Xu</u> and Akira Onoda, "Accurate and Fast Prediction of Protein pK_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]

- <u>Shijie Xu</u> 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]

- <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

- Recipient of the Outstanding Student Scholarship, University of Science and Technology of China, 2016

- S.-T. Yau College Student Mathematics Contest, Beijing, China, 2016

- Recipient of the Outstanding Freshman Scholarship, University of Science and Technology of China, 2014

- Winner of the First Prize in the National High School Mathematics League (province level), Hefei, Anhui, China, 2012