

# CURRICULUM VITAE

## Shijie Xu

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### Date of Birth

March 9th, 1995

### Education

Ph.D. in Environmental Science, Hokkaido University	March 2025
<i>Dissertation Title: "Accurate and Fast Predictions of Protein Structures and Properties via Protein Language Models"</i>	
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
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### Research Interests

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

### Skills

**Programming:** Python / C++ /  $\text{\LaTeX}$  / 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 (standard and lower Yangtze)

### Publications

1. [Shijie Xu](#) and Akira Onoda\*. "Probe-Based Identification of Metal-Binding Sites Using Deep Learning Representations." *Under Review*, **2025**.
2. [Shijie Xu](#) and Akira Onoda\*. "Accurate and Rapid Prediction of Protein  $\text{pK}_a$ : Protein Language Models Reveal the Sequence- $\text{pK}_a$  Relationship." *Journal of Chemical Theory and Computation* 21(7): 3752–3764, **2025**, DOI: <https://doi.org/10.1021/acs.jctc.4c01288>

3. [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>
4. [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, **2024**, DOI: <https://doi.org/10.1021/acs.jcim.3c01202>

## Presentations

- [Shijie Xu](#) 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]
- [Shijie Xu](#) 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]
- [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
- 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, Hefei, Anhui, China, 2012