

Ailun (Ellen) Wang

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[g](#) Ailun Wang

Education

Boston College

Ph.D., Computational Biophysics

Chestnut Hill, MA

Aug. 2015 - June 2021

University of Science and Technology of China (USTC)

B. Sc., Materials Chemistry

Hefei, China

Aug. 2011 - July 2015

Professional Experience

Northeastern University

Postdoctoral Fellow at Center for Theoretical Biological Physics (CTBP)

Boston, MA

July 2021 - present

Research Experience

Highlights: Molecular modeling; High-performance computing; Large-scale data analysis; Advanced data visualization; Statistical modeling.

Prediction of antigen recognition on T-cell receptors using Machine Learning-based classification

Northeastern University, CTBP, 2021–present

- Developed a physical model in Python for predicting binding specificity between T-cell receptors (TCR) and antigens.
- Utilized a Machine Learning based method to classify contact interfaces in strongly vs. weakly binding TCR and antigens.
- Achieved high transferability and sensitivity with 94% accuracy on blind test cases.

Constructing 3D architecture of chromatin at high resolution

Northeastern University, CTBP, 2021–present

- Designed a transferable model for predicting 3D architecture of chromatin to investigate the structural features of gene.
- Implemented physical models for molecular dynamics (MD) simulations in Python and optimized model parameters to align with experimental measurements.
- Predicted the 3D architectures of chromatin segments that closely agree with experimental measurements and the manuscript is currently under review.

Demystify the effect of ions in conformational dynamics of ribosome using computational methods

Boston College, 2016-2021

- Developed a force field to facilitate MD simulations of large biomolecules (sub-million atoms) with ions.
- Implemented an iterative parameter optimization protocol in Python and C++ for force field development.
- Conducted long-timescale MD simulations on HPC clusters and analyzed structural features using statistical methods in Python from terabytes of raw data.
- Provided the first computational explanation of how diffuse Mg^{2+} and K^{+} ions regulate large-scale conformational rearrangements of ribosome.
- Published 6 peer-reviewed journal articles and 1 book chapter and presented at 8 conferences.

Theoretical investigation of ion transportation mechanism in porous materials

Boston College, 2019-2020

- Illustrated the ion transport mechanism in porous materials using density functional theory (DFT) calculations and *ab initio* MD simulations in multi-disciplinary collaboration with materials science experimentalists.
- Published 2 peer-reviewed journal articles.

Selected Honors and Awards

2020: Engelhard Pingree Research Fellowship

Boston College

2019: IHPCCS Fastest CPU Code

International HPC Summer School (IHPCCS) 2019

2013: Outstanding Student Scholarship

USTC

Technical Skills

Languages & Platforms: Python, Shell Script, SQL, Mathematica, Matlab, C++, \LaTeX , Linux/Unix, Slurm, HPC

Softwares & Packages: Git, Jupyter notebook, Pandas, NumPy, SciPy, Seaborn, Plotly, scikit-learn, Gromacs, OpenMM, Amber, Modeller, Rosetta, VMD, Chimera, Schrödinger, Quantum Espresso

Publications

Peer Reviewed Articles

- Gu, H., Harris, H. L., Olshansky, M., **Wang, A.**, et al. (2023). Chromatin Alternates Between A and B Compartments at Kilobase Scale for Subgenomic Organization. *Nature Communications* (in press).
- Wang, Y., **Wang, A.**, Mohanty, U., Whitford, P. C. (2022). Precise Steric Features Control Aminoacyl-tRNA Accommodation on the Ribosome. *The Journal of Physical Chemistry B*, 126(42), 8447–8459.
- **Wang, A.**, Levi, M., Mohanty, U., Whitford, P. C. (2022). Diffuse Ions Coordinate Dynamics in a Ribonucleoprotein Assembly. *Journal of The American Chemical Society*, 144(21), 9510–9522.
- De Oliveira Jr, A. B., Contessoto, V. G., Hassan, A., Byju, S., **Wang, A.**, Wang, Y., Dodero-Rojas, E., Mohanty, U., Noel, J. K., Onuchic, J. N., Whitford, P. C. (2022). SMOG 2 and OpenSMOG: Extending the limits of structure-based models. *Protein Science*, 31(1), 158-172.
- Wang, Y., Luo, T., Li, Y., **Wang, A.**, Wang, D., Bao, J. L., Mohanty, U., Tsung, C.-K. (2021). Molecular-Level Insights into Selective Transport of Mg^{2+} in Metal–Organic Frameworks. *ACS Applied Materials & Interfaces*, 13(44), 51974-51987.
- Levi, M., Walak, K., **Wang, A.**, Mohanty, U., Whitford, P. C. (2020). A Steric Gate Controls P/E Hybrid-state Formation of tRNA on the Ribosome. *Nature Communications*, 11(1), 1-12.
- Luo, J., Li, Y., Zhang, H., **Wang, A.**, Lo, W.-S., Dong, Q., Wong, N., Povinelli, C., Shao, Y., Cherreddy, S., Wunder, S., Mohanty, U., Tsung, C.-K., Wang, D. (2019). A Metal-Organic Framework Thin Film for Selective Mg^{2+} Transport. *Angewandte Chemie International Edition*, 58(43), 15313-15317.
- Hutchison, C., Bhattarai, A., **Wang, A.**, Mohanty, U. (2019). Fluctuation Effects in the Adam-Gibbs Model of Cooperative Relaxation. *The Journal of Physical Chemistry B*, 123(38), 8086-8090.
- Lammert, H., **Wang, A.**, Mohanty, U., Onuchic, J. N. (2018). RNA as a Complex Polymer with Coupled Dynamics of Ions and Water in the Outer Solvation Sphere. *The Journal of Physical Chemistry B*, 122(49), 11218-11227.
- Wang, L., Ge, J., **Wang, A.**, Deng, M., Wang, X., Bai, S., Li, R., Jiang, J., Zhang, Q., Luo, Y., Xiong, Y. (2014). Designing p-type Semiconductor-metal Hybrid Structures for Improved Photocatalysis. *Angewandte Chemie International Edition*, 126(20), 5207-5211.

Book Chapter

- Levi, M., Bandarkar, P., Yang, H., **Wang, A.**, Mohanty, U., Noel, J. K., & Whitford, P. C. (2019). Using SMOG 2 to Simulate Complex Biomolecular Assemblies. *Biomolecular Simulations: Methods and Protocols* (pp. 129-151).

Selected Presentations

2023: Contributed poster presentation, 67th Biophysical Society Annual Meeting, San Diego, CA

2021: Contributed poster presentation, 35th Annual Gibbs Conference on Biothermodynamics, Virtual

2020: Invited talk, Graduate Student Symposium, Dept. of Chemistry, Boston College, Chestnut Hill, MA

2019: Selected talk, Molecular Biophysics in the Northeast 2019, Boston, MA

2019: Contributed talk, APS March Meeting, Boston, MA

2018: Contributed poster presentation, 256th ACS National Meeting, Boston, MA