# Ailun (Ellen) Wang

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Ailun Wang

## Education

**Boston College** — **Chestnut Hill, MA**
*Ph.D. in Physical Chemistry* — *Aug. 2015 - June 2021*

**University of Science and Technology of China (USTC)** — **Hefei, China**
*B. Sc. in Materials Chemistry* — *Aug. 2011 - July 2015*

## Professional Experience

**Northeastern University** — **Boston, MA**
*Postdoctoral Fellow at Center for Theoretical Biological Physics (CTBP)* — *July 2021 - July 2023 (expected)*

## Research Experience

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

**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.

**Demystify the effect of ions in conformational dynamics of ribosome using computational methods**
*Boston College, 2016-2021*

- Developed an implicit solvent force field to facilitate MD simulations of a full ribosome (sub-million atoms) with explicit 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.
- The force field parameters are publicly available on SMOG-server with both Gromacs and OpenMM suport.
- 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**: IHPCSS Fastest CPU Code *International HPC Summer School (IHPCSS) 2019*

## Technical Skills

**Languages & Platforms**: Proficient in Python, Shell Script, Linux/Unix, Slurm, familiar with HPC, C++, SQL, Mathematica, Matlab

**Softwares & Tools**: Git, Jupyter notebook, Pandas, NumPy, SciPy, Seaborn, Plotly, Gromacs, OpenMM, Amber, Modeller, Rosetta, VMD, Chimera, Maestro, 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 Subgenic 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.,Chereddy, 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, Catalyzing Gender Equity Event at Schrödinger, Inc., *New York, NY*

**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*