

Ailun (Ellen) Wang

☎ 617-909-5120 • ✉ ellenfidele@gmail.com • 🌐 ailun-wang • 📧 ellenfidele

Education

Boston College

Ph.D. in Chemistry

Areas of Expertise: Computational Biophysics, Molecular Dynamics, RNA, Protein, High Performance Computing

Chestnut Hill, MA

Aug. 2015 - June 2021

University of Science and Technology of China (USTC)

B. Sc. in 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

Northeastern University, CTBP

Postdoctoral Fellow

Boston, MA

July 2021 - present

- Optimized a predictive model using sequences and structures of T-cell receptors (TCR) and antigen peptides for investigating the antigen binding specificities and predicting the **antigen recognition** of TCR.
- Developed a transferable physical model in **Python** for predicting 3D architectures of chromatin using molecular dynamics (MD) simulations with OpenMM on **high performance computing (HPC)** clusters.

Boston College

Research Associate

Chestnut Hill, MA

Aug. 2015 - June 2021

- Developed a **force field** for MD simulations of large biomolecules (sub-million atoms) with explicit ions by integrating electrostatics interactions and ion hydration effects into an implicit solvent model.
- Implemented automated iterative **parameter optimization** protocols for force field development.
- Provided the first computational explanation of how diffuse Mg^{2+} and K^+ ions regulate **large-scale conformational rearrangements** of ribosome using long timescale MD simulations.
- Illustrated the ion transport mechanism in porous materials using density functional theory calculations and *ab initio* MD simulations in **multi-disciplinary collaboration** with materials science experimentalists.

Publications

Peer Reviewed Articles

- 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* (in press, DOI: 10.1021/acs.jpcb.2c05513).
- **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. In *Biomolecular Simulations* (pp. 129-151). Humana, New York, NY.

Manuscript In Preparation.....

- Gu, H., Harris, H. L., Olshansky, M., **Wang, A.**, *et al.* (2022). Chromatin alternates between A and B compartments at kilobase scale for subgenomic organization. (*Submitted to Nature Genetics*. Latest preprint: <http://dx.doi.org/10.2139/ssrn.4138705>)

Presentations

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*

2019: Contributed poster presentation, International HPC Summer School, *Kobe, Japan*

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

2018: Contributed poster presentation, Cokerfest symposium, *Boston, MA*

2016: Contributed poster presentation, Greater Boston Area Statistical Mechanics Meeting, *Waltham, MA*

Selected Honors and Awards

2020: Engelhard Pingree Research Fellowship

Boston College

2019: IHPCSS Fastest CPU Code

International HPC Summer School 2019

2013: Outstanding Student Scholarship

USTC

2013: Sun Guo-sheng Leadership Scholarship

USTC

Technical Skills

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

Softwares & Tools: Git, Jupyter notebook, Pandas, NumPy, SciPy, Gromacs, OpenMM, Amber, Modeller, VMD, Chimera, Maestro, Quantum Espresso