

Ailun (Ellen) Wang

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Education

Boston College

Ph.D. in Physical Chemistry

Areas of Expertise: Computational Biophysics, Python, Data Analysis, High Performance Computing, Predictive Model, Data Visualization.

University of Science and Technology of China (USTC)

B. Sc. in Materials Chemistry

Chestnut Hill, MA

Aug. 2015 - June 2021

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: High-performance scientific 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

- 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

- 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

- 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

- 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-review 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

Programming: Python (7 years), Shell Script, SQL, Mathematica, Matlab, C++, \LaTeX

Softwares & Tools: Linux/Unix, Git, HPC, OpenMP, MPI, Jupyter notebook, Pandas, NumPy, SciPy, Matplotlib, Seaborn, Plotly