

# Chuankai Zhao

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## EXECUTIVE SUMMARY

- Seeking a **Software Engineering Intern** position for the **summer 2019**.
- Ph.D. candidate, multidisciplinary computational researcher with strong analytical, problem-solving skills.
- Experienced in Python/C/C++, parallel computing, large-scale data analysis and machine learning.
- Proven record of interdisciplinary collaboration, team work, strong written & verbal communication skills.

## EDUCATION

**Ph.D., Chemical & Biomolecular Engineering**, University of Illinois at Urbana-Champaign, 2015-2020  
• Advisor: Prof. Diwakar Shukla; GPA: 3.9/4.0; Concentration: **Computational Science & Engineering**

**M.S., Chemical & Biomolecular Engineering**, University of Illinois at Urbana-Champaign, 2015-2018

**B.S., Materials Science & Engineering**, Shanghai Jiao Tong University, 2011-2015

## SKILLS

**Technical skills:** Modeling & simulation, Markov state model, Statistics, Machine learning, Deep learning, Data analysis, Scientific visualization, Algorithms, Data structures, Bioinformatics, Cheminformatics, Computer-aided design, High-performance computing, GPU programming, Web development

**Programming:** Python, C/C++, CUDA C, shell scripting, SQL, JavaScript, HTML, MATLAB

**Softwares:** TensorFlow, Scikit-learn, Keras, Git, L<sup>A</sup>T<sub>E</sub>X, Microsoft office, NumPy, Pandas, Matplotlib, D3.js

**Soft skills:** Interdisciplinary collaboration, Multitasking and planning, Team work, Time management, Effective communication, Decision making, Leadership, Self-motivation, Optimism, Enthusiasm, Self-confidence

## RESEARCH EXPERIENCE

**Graduate Research**, University of Illinois at Urbana-Champaign, Aug 2015-

- **Revealing the Molecular Mechanisms of Plant Hormone Signaling (ongoing work)**
  - Performed large-scale molecular dynamics and kinetic Monte Carlo simulations on petascale supercomputing facility to unravel complete perception mechanisms of 7 key plant hormones.
  - Constructed Markov models to analyze time series data from simulations and quantitatively characterized high-dimensional dynamics, thermodynamics and kinetics of hormone perceptions.
  - Employed genetic algorithm and dimensionality reduction techniques in feature search/selection, and utilized variational cross-validation to optimize parameters for model constructions.
  - Utilized statistical and numerical methods to quantify solvation thermodynamics of receptor proteins, and thermodynamic profiles of protein-protein associations involved in hormone signaling.
- **Agrochemical Discovery using Machine Learning (ongoing work)**
  - Trained deep neural network (DNN) models to predict agrochemical-likeness of small molecules.
  - Trained DNN models to classify different types of agrochemicals and define agrochemical space.
  - Compared task prediction accuracy of DNN models with random forest and support vector machine.
- **Neural Network-based Enhanced Sampling for Biomolecular Simulations (ongoing work)**
  - Developing deep learning models to identify reaction coordinates for enhanced sampling techniques.
  - Implementing neural network-based enhanced sampling algorithms in NAMD simulation software.
- **Development of Experiment-guided Sampling Method for Large-scale Molecular Simulations**
  - Proposed the efficient sampling algorithm to explore protein conformational space by combining Markov chain adaptive sampling with computational and experimental data.
  - Implemented the algorithm and demonstrated applications in modeling protein/complex structures.
- **Quantifying the Effects of Divalent Cations on TALE DNA-Binding Specificity**
  - In collaboration with Profs. Charles Schroeder and Huimin Zhao Groups at Illinois.

- Identified the presence of divalent cations as key to achieving TALE specificity for precise gene editing.
- Developed thermodynamic models to quantitatively characterize TALE-DNA binding free energy changes in various salt solutions, and unraveled molecular origins of divalent cation effects.
- **Dynamic-Template-Directed Multiscale Assembly for Coating of Polymer Thin Films**
  - In collaboration with Prof. Ying Diao Group at Illinois.
  - Designed the ionic-liquid-based dynamic templates to expedite polymer nucleation and ensuing assembly process during solution coating to prepare highly-aligned polymer thin films.
  - Demonstrated the surface reconfigurability of template as key to promoting template-polymer interactions, thereby lowering polymer nucleation barrier via molecular modeling.

## SOFTWARE ENGINEERING EXPERIENCE

- **CS 483, Applied Parallel Programming**, University of Illinois, Fall 2018 (ongoing work)
  - Designed and implemented neural network convolutional layer forward pass using CUDA C.
  - Utilized NVIDIA Visual Profiler to analyze and optimize kernel performance in image recognitions.
- **CS 519, Scientific Visualization**, University of Illinois, Fall 2017
  - Developed the webserver WaterBank (<https://github.com/chuankaizhao/WaterBank>) to visualize global drought conditions based on historical water resources/uses data acquired from AQUASTAT database.

## PUBLICATIONS & CONFERENCES

Peer-reviewed research articles: **4 published/accepted, 2 under review, 3 in preparation.**

Contributed to **9 research presentations in national and regional conferences.**

1. Mohammadi E., **Zhao C.**, et al. (2018). Ion Gel Dynamic Templates for Enhanced Semiconducting Polymers Morphological and Electrical Characteristics. **J. Am. Chem. Soc.**, under review.
2. Cuculis L.\*, **Zhao C.\***, Abil Z., Zhao H., Shukla D. and Schroeder C.M. (2018). Divalent Cations Enhance TALE DNA-binding Specificity. **Angew. Chem. Int. Ed.**, under review. (\* denotes **co-first** author)
3. Shukla S.\*, **Zhao C.\*** and Shukla D. (2018). Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. **Structure**, in press. (\* denotes **co-first** author)
4. **Zhao C.** and Shukla D. (2018). SAXS-guided Enhanced Unbiased Sampling for Structure Determination of Proteins and Complexes. **Sci. Rep.**, in press.
5. Mohammadi E., **Zhao C.**, et al. (2017). Dynamic-Template-Directed Multiscale Assembly for Large-Area Coating of Highly-Aligned Conjugated Polymer Thin Films. **Nat. Commun.**, 8, 16070. (**Highlighted on Illinois homepage, Science Magazine, EurekAlert!, Science Daily, Phys.org, etc.**)
6. Ni Z., Liu J., Wu Y., Liu B., **Zhao C.**, et al. (2015). Fabrication of Platinum Submonolayer Electrodes and Their High Electrocatalytic Activities for Ammonia Oxidation. **Electrochim. Acta**, 177, 30-35.

## HONORS & AWARDS

- Popular Choice Poster Award, Biophysics Graduate Symposium, University of Illinois, 2018
- Hamratty Travel Award, University of Illinois at Urbana-Champaign, 2018
- 3M Corporate Fellowship, University of Illinois at Urbana-Champaign, 2018-2019
- List of Excellent Teachers, University of Illinois at Urbana-Champaign, 2017
- Outstanding Graduate Award (**top 5%**), Shanghai Jiao Tong University, 2015
- National Endeavor Scholarship (**top 5%**), Shanghai Jiao Tong University, 2015
- Overseas Study Scholarship (**first class, 1%**), Shanghai Jiao Tong University, 2014
- Liu Garden Scholarship (**top 5%**), Shanghai Jiao Tong University, 2013
- Academic Excellence Scholarship (**top 5%**), Shanghai Jiao Tong University, 2012, 2013, 2014
- Excellent Project Award, Undergraduate Innovation Program, Shanghai Jiao Tong University, 2014

## PROFESSIONAL ACTIVITIES

- **Graduate Mentor**, Illinois Scholars Undergraduate Research Program, University of Illinois, 2016-2017
- **Entrepreneurship Summer Program**, National University of Singapore, July 2014
- **Teaching Assistants**: Process Design, Process Control, Heat & Mass Transfer (graduate level), 2016-2018
- **Lab Instructor**: GAMES Camps, Girls Adventures in Math, Engineering, and Science, Illinois, 2016-2018