

# Chuankai Zhao

## CONTACT INFORMATION

293 RAL, 600 S Mathews Ave  
Urbana, IL 61801

[czhao37@illinois.edu](mailto:czhao37@illinois.edu)  
<http://go.illinois.edu/zhao>

## EDUCATION

- Ph.D.**, Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign 2015-2020
- Concentration: Computational Science & Engineering
  - Advisor: Professor Diwakar Shukla
- M.S.**, Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign 2015-2018
- B.S.** (with Honors), Materials Science & Engineering, Shanghai Jiao Tong University 2011-2015
- Thesis: *Ab initio* study of the ideal tensile and shear strength of B2 CuZr
  - Advisor: Professor Lingti Kong and Professor Cheng Zhong

## RESEARCH EXPERIENCE

**Graduate Research**, University of Illinois at Urbana-Champaign 2015/10-Present

- **Revealing the Molecular Mechanisms of Plant Hormone Signaling**
  - Performed large-scale molecular dynamics (~1 millisecond aggregate) and Monte Carlo simulations on 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 and 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**
  - 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.
- **Experimental-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 Professors 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 Professor 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.

Undergraduate Research, Shanghai Jiao Tong University

2012/09-2015/07

- **First Principle Study of the Ideal Strength of B2 CuZr**
  - Calculated the elastic constants and plotted the 3D anisotropic diagrams of elastic modulus.
  - Investigated the B2 CuZr response behaviors under tensile loading and shear loading.
- **Fabrication of Pt Monolayer Electrode for Electrocatalytic Ammonia Oxidation**
  - Designed the Pt monolayer coated electrode via underpotential deposition and redox replacement.
  - Demonstrated the high electrocatalytic efficiency of Pt monolayer electrode in ammonia oxidation.
  - Won the Excellent Project Award of Undergraduate Innovation Program.

## HONORS & AWARDS

- Popular Choice Poster Award, Biophysics Graduate Symposium, University of Illinois 2018
- Hanratty 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 2012-2014
- Excellent Project Award, Undergraduate Innovation Program, Shanghai Jiao Tong University 2014
- Maohua Scholar (undergraduate tuition fully covered), Maohua Charitable Foundation 2011-2015

## PUBLICATIONS

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. DOI: 10.1016/j.str.2018.12.005. (\* 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.**, 8, 17748.
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.

## ORAL PRESENTATIONS

1. **Zhao C.** (2018). Structural, dynamic and energetic basis of plant hormone signal transduction. Photosynthesis Research Unit Seminar, University of Illinois at Urbana-Champaign, Urbana, IL.
2. **Zhao C.** (2018). Dewetting controls plant hormone perception and initiation of drought resistance sig-

ning. 17<sup>th</sup> Annual Graduate Research Symposium, Chemical and Biomolecular Engineering at Illinois, Urbana, IL.

3. Mohammadi E., **Zhao C.**, Meng Y., Mei J., Zuo J., Shukla D. and Diao Y. (2017). Surface-directed assembly for large-area coating of highly-aligned conjugated polymer thin films. 253<sup>rd</sup> ACS National Meeting, San Francisco, CA.
4. Selvam B., Mittal S., **Zhao C.** and Shukla D. (2016). Design of optimal experimental probes for protein dynamics using machine learning and variational approach to modeling conformational kinetics. AIChE Annual Meeting, San Francisco, CA.

## POSTER PRESENTATIONS

1. **Zhao C.** and Shukla D. (2018). Complex dynamics of hormone perception and receptor activation in plant drought resistance signaling. 256<sup>th</sup> ACS National Meeting, Boston, MA.
2. **Zhao C.** and Shukla D. (2018). Computational investigation into the activation of abscisic acid signaling for drought stress responses in plants. Plant Molecular Biology Gordon Research Conference, Holderness, NH.
3. **Zhao C.**, Meigooni M. and Shukla D. (2017). How do plants perceive hormones to activate drought resistance signaling? Monsanto Research Symposium, University of Illinois at Urbana-Champaign, Urbana, IL.
4. Meigooni M., **Zhao C.** and Shukla D. (2017). Elucidating binding mechanisms of ABA analogues: Activation of PYL5 receptor by pyrabactin and quinabactin. 253<sup>rd</sup> ACS National Meeting, San Francisco, CA.
5. Shukla S., Meigooni M., **Zhao C.** and Shukla D. (2017). Machine learning guided ligand-protein simulation approach elucidates the binding mechanism of abscisic acid. 61<sup>st</sup> Annual Biophysical Society Meeting, New Orleans, LA.
6. Shamsi Z., Shukla S., **Zhao C.** and Shukla D. (2016). Markov state models provide insights into dynamic modulation of protein function. AIChE Annual Meeting, San Francisco, CA.

## TEACHING EXPERIENCE

- Teaching Assistant, Process Design (ChBE 431), Fall 2016, University of Illinois
- Teaching Assistant, Process Control (ChBE 440), Spring & Fall 2017, University of Illinois
- Teaching Assistant, Heat & Mass Transfer (ChBE 523, graduate course), Spring 2018, University of Illinois

## MENTORING EXPERIENCE

Graduate mentor for the following undergraduate students at the University of Illinois:

- Aik Rui Tan, MatSE 2019 Class, currently applying for graduate school 2018/05-Present
- Moeen Meigooni, ChBE 2017 Class, currently Ph.D. student at University of Illinois. 2016/09-2017/05

## PROFESSIONAL EXPERIENCE

- Reviewer for **Z. Anorg. Allg. Chem.** and co-reviewer for **J. Chem. Phys.**, **J. Phys. Chem. B.**
- **Entrepreneurship Summer Program**, National University of Singapore, 2014/07

## TECHNICAL STRENGTH

- **Technical skills**
  - Expertized in molecular dynamics (MD) & Monte Carlo simulations, biased sampling methods including metadynamics, umbrella sampling and replica-exchange MD, as well as alchemical free energy methods.
  - Experienced in Markov modeling on time series data from long timescale molecular simulations.

- Experienced in high performance computing, data analysis, statistical modeling and data visualization.
- Familiar with machine learning and deep learning algorithms as well as their applications in molecular simulations and drug discovery.
- Familiar with theory and tools of bioinformatics and cheminformatics.
- Familiar with algorithms and data structures, and exposure to web development and visualization.
- **Programming**
  - Experienced in Python, C/C++, shell scripting, SQL.
  - Familiar with GPU programming, CUDA and OpenACC.
  - Exposure to JavaScript, HTML, MATLAB.
- **Softwares**
  - **Modeling:** Amber, OpenMM, NAMD, Gromacs, VASP, Schrodinger, AutoDock, Rosetta, Chimera
  - **Data analysis:** NumPy, SciPy, Pandas, MDTraj, MSMBuilder, Osprey
  - **Visualization:** PyMOL, VMD, Matplotlib, D3.js, Origin
  - **Machine learning:** Scikit-learn, TensorFlow, Keras, MXNet, DeepChem
  - **Others:** Git, LATEX, Microsoft office, MATLAB, Octave
- **Soft skills:** Interdisciplinary collaboration, Multitasking and planning, Team work, Time management, Effective communication, Decision making, Self-motivation, Optimism, Enthusiasm, Self-confidence

## OUTREACH ACTIVITIES

- **GAMES Camps, Girls' Adventures in Math, Engineering, and Science**, Illinois 2016-2018
  - Organized activities related to computational investigations of protein structure & function.
- **Mainland-Taiwan College Students Summer Camp**, Shanghai Jiao Tong University 2013/07
  - Organized the two-week camp events including lectures, discussions and field exploration.
- **Volunteer Teaching in Jiujiang Yang Guang Middle School**, Jiangxi, China 2012/07
  - Co-led a team of 17 undergraduate volunteers to teach extracurricular courses in the rural school.