

# Curriculum Vitae: Chuankai Zhao

## CONTACT INFORMATION

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## EDUCATION

- **Ph.D.**, Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign 2020
  - **Graduate Concentration:** Computational Science & Engineering
  - Advisor: Professor Diwakar Shukla (<http://shuklagroup.org>)
- **M.S.**, Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign 2018
- **B.S.** (with Honors), Materials Science & Engineering, Shanghai Jiao Tong University, China 2015
  - Thesis: Density Functional Theory Study of the Ideal Strength of B2 CuZr
  - Advisor: Professor Lingti Kong (<https://nes.sjtu.edu.cn/english.htm>)
- **Summer Program**, Entrepreneurship, National University of Singapore 2014

## RESEARCH INTERESTS

- High-performance computing for computational chemistry, biophysics and materials science
- Modeling and simulation of polymers, protein-ligand binding, protein-protein and protein-DNA interactions
- Statistical modeling of high-dimensional, large-scale time series molecular simulation datasets
- Computational method and software development for efficient sampling in molecular simulations
- Machine learning for small molecular discovery and computer-aided, structure-based molecular design

## HONORS & AWARDS

- Glenn E. and Barbara R. Ullyot Graduate Fellowship, University of Illinois 2019-2020
- Outstanding Student Research Award, GLCACS 23<sup>rd</sup> Annual Conference 2019
- **First Prize**, Science & Spirits Poster Competition, University of Illinois at Urbana-Champaign 2019
- 3M Corporate Fellowship, University of Illinois at Urbana-Champaign 2018-2019
- Popular Choice Poster Award, Biophysics Graduate Symposium, University of Illinois 2018
- Hanratty Travel Award, University of Illinois at Urbana-Champaign 2018
- 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
- Maohua Scholar (undergraduate tuition fully covered), China Maohua Foundation 2011-2015
- Overseas Study Scholarship (**first class, 1%**), Shanghai Jiao Tong University 2014
- Academic Excellence Scholarship (**top 5%**), Shanghai Jiao Tong University 2012-2014
- Excellent Project Award, Undergraduate Innovation Program, Shanghai Jiao Tong University 2014
- Liu Garden Scholarship (**top 5%**), Shanghai Jiao Tong University 2013

## PUBLICATIONS

1. Aldukhi F.<sup>†</sup>, Deb A.<sup>†</sup>, **Zhao C.**, Moffett A.S. and Shukla D. (2019). Molecular Mechanism of Brassinosteroids Perception by the Plant Growth Receptor BRI1. **Journal of Physical Chemistry B**, minor revision invited. († denotes **co-first** author)
2. **Zhao C.** and Shukla D. (2019). Molecular Basis of the Activation and Dissociation of Dimeric PYL2 Receptor in Abscissic Acid Signaling. **Chemical Science**, revision invited. (bioRxiv DOI: 10.1101/721761)
3. Cuculis L.<sup>†</sup>, **Zhao C.**<sup>†</sup>, Abil Z., Zhao H., Shukla D. and Schroeder C.M. (2019). Divalent Cations Promote TALE DNA-binding Specificity. **Nucleic Acids Research**, minor revision invited. († denotes **co-first** author)
4. Mohammadi E., **Zhao C.**, Zhang F., Qu G., Jung S.-H., Lee J.-K., Zhao Q., Evans C., Lee J.-K., Shukla D. and Diao Y. (2019). Ion Gel Dynamic Templates for Large Modulation of Morphology and Charge Transport Properties of Solution-Coated Conjugated Polymer Thin Films. **ACS Applied Materials & Interfaces**, 11, 22561-22574.
5. Shukla S.<sup>†</sup>, **Zhao C.**<sup>†</sup> and Shukla D. (2019). Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. **Structure**, 27, 692-702.e3. († denotes **co-first** author)
6. **Zhao C.** and Shukla D. (2018). SAXS-guided Enhanced Unbiased Sampling for Structure Determination of Proteins and Complexes. **Scientific Reports**, 8, 17748.
7. Mohammadi E., **Zhao C.**, Meng Y., Qu G., Zhang F., Zhao X., Mei J., Zuo J., Shukla D. and Diao Y. (2017). Dynamic-Template-Directed Multiscale Assembly for Large-Area Coating of Highly-Aligned Conjugated Polymer Thin Films. **Nature Communications**, 8, 16070. (Highlighted on Illinois homepage, Science Magazine, EurekAlert!, Science Daily, Phys.org, etc.)
8. Ni Z., Liu J., Wu Y., Liu B., **Zhao C.**, Deng Y., Hu W. and Zhong C. (2015). Fabrication of Platinum Sub-monolayer Electrodes and Their High Electrocatalytic Activities for Ammonia Oxidation. **Electrochimica Acta**, 177, 30-35.

## ORAL PRESENTATIONS

1. **Zhao C.**, Chen J., Aldukhi F., Moffett A.S. and Shukla D. (2019). Quantitative characterization of protein-ligand and protein-protein binding processes involved in plant hormone signaling. AICHE Annual Meeting, Orlando, FL.
2. **Zhao C.** and Shukla D. (2019). Molecular basis and engineering of plant drought resistance signaling. Great Lakes Chinese American Chemical Society 23<sup>rd</sup> Annual Conference, Chicago, IL.
3. **Zhao C.** and Shukla D. (2019). Molecular basis and engineering of plant drought resistance signaling. Science & Spirits Lightning Talks, University of Illinois, Urbana, IL. (invited)
4. **Zhao C.** and Shukla D. (2018). Structural, dynamic and energetic basis of plant hormone signal transduction. Photosynthesis Research Unit Seminar, University of Illinois, Urbana, IL.
5. **Zhao C.** and Shukla D. (2018). Dewetting controls plant hormone perception and initiation of drought resistance signaling. 17<sup>th</sup> Annual Graduate Research Symposium, Chemical and Biomolecular Engineering at Illinois, Urbana, IL.
6. 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.
7. 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. (2019). Towards rational design of chemical modulators to improve plant drought tolerance. AIChE Annual Meeting, Orlando, FL.
2. **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.
3. **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.
4. **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.
5. 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.
6. 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.
7. 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.

## RESEARCH EXPERIENCE

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

2015/10-Present

- **Molecular & Statistical Modeling of the Molecular Mechanisms of Plant Hormone Signaling (ongoing)**
  - Performed large-scale all-atom molecular dynamics simulations on petascale supercomputer to unravel the molecular mechanisms of ligand binding and subsequent receptor activation for 7 key plant hormones.
  - Constructed Markov state models to analyze time series simulation data and quantitatively characterized high-dimensional long timescale dynamics, thermodynamics and kinetics of plant hormone perceptions.
  - Employed genetic algorithm and dimensionality reduction techniques in feature search and selection, and utilized variational cross-validation to optimize parameters for Markov model constructions.
  - Related publications: Shukla<sup>†</sup>, Zhao<sup>†</sup> and Shukla, Structure, 2019; Zhao and Shukla, 2019 (in review); Aldukhi<sup>†</sup> and Deb<sup>†</sup> *et al.*, 2019 (in review).
- **Quantitative Characterization of Effects of Plant Hormone Binding on Protein-Protein Association**
  - Performed replica-exchange umbrella sampling simulations to characterize the effects of plant hormone binding on protein-protein interactions involved in plant hormone signaling (molecular glue hypothesis).
  - Constructed protein-protein association free energy profiles using Multistate Bennett Acceptance Ratio (MBAR) method, allowing for quantitative characterization of plant hormone binding effects.
  - Related publication: Zhao and Shukla, 2019 (in review).
- **Machine Learning for Agrochemical Activity Prediction & Discovery (ongoing)**
  - Extracted and cleaned crop protection agrochemical activity data from the ChemBL database using Python and SQL, and featurized the molecules (>40,000) using molecular fingerprints via Python RDKit.
  - Trained random forest, gradient boosting, and neural network multi-class classification models using Scikit-Learn and Keras to predict small molecule agrochemical-likeness, achieving ~80% accuracy.
  - Related publication: Tan, Zhao and Shukla, 2019 (in preparation).

- **Experimental-guided Sampling Method for Large-scale Molecular Simulations**

- Designed an efficient Markov-chain-based statistical sampling algorithm with sparse experimental data incorporated to guide iterative unbiased molecular simulation and predict accurate biomolecule ensemble.
- Implemented the algorithm with Python and demonstrated in studying protein folding and protein-protein association processes, leading to >50% reduction in required computational time and 1 publication.
- Related publication: Zhao and Shukla. Sci. Rep., 2018.

- **NAMD Software Development for Implementation of Deep Learning Based Sampling (ongoing)**

- Surveyed the literatures on utilizing variational autoencoder and reinforcement learning to identify low-dimensional reaction coordinates for efficient enhanced sampling in molecular dynamics simulations.
- Designed and implementing the software architecture to interface NAMD, a popular molecular simulation package (C++), with Python deep learning frameworks to support data-driven sampling techniques.

- **Quantifying the Effects of Divalent Cations on TALE DNA-Binding Specificity**

- In cross-functional 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 characterize TALE-DNA binding free energy changes in various salt solutions based on molecular simulations, and unraveled molecular origins of divalent cation effects.
- Related publications: Cuculis<sup>†</sup> and Zhao<sup>†</sup> *et al.* 2019 (in review).

- **Dynamic-Template-Directed Multiscale Assembly for Coating of Polymer Thin Films**

- In cross-functional collaboration with Professor Ying Diao Group at Illinois.
- Designed the ionic-liquid-based and the ion-gel-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.
- Related publications: Mohammadi *et al.* Nat. Commun., 2017; ACS Appl. Mater. Interfaces, 2019.

**Undergraduate Research**, Shanghai Jiao Tong University

2012/09-2015/07

- **First Principle Study of the Ideal Strength of B2 CuZr**

- Calculated elastic constants and 3D elastic modulus of B2 CuZr alloy using density functional theory.
- Investigated the B2 CuZr mechanical response behaviors under tensile loading and shear loading.

- **Fabrication of Pt Monolayer Electrode for Electrocatalytic Ammonia Oxidation**

- Designed Pt monolayer coated electrode via underpotential deposition and redox replacement.
- Demonstrated high electrocatalytic efficiency of Pt monolayer electrode in ammonia oxidation.
- Related publication: Ni *et al.* Electrochim. Acta, 2015.

## **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:

- Aniket Deb, summer student research intern from Jadavpur University, India
- Faisal Aldukhi, ChBE'19, currently M.S. student at King Abdullah University of Science and Technology
- Aik Rui Tan, MatSE'19, currently Ph.D. student at Massachusetts Institute of Technology
- Moeen Meigooni, ChBE'17, currently Ph.D. student at University of Illinois

## PROFESSIONAL EXPERIENCE

- Journal reviewer for Zeitschrift fur anorganische und allgemeine Chemie, Journal of Chemical Physics, Journal of Physical Chemistry B, Journal of Chemical Information and Modeling

## RESEARCH COLLABORATORS

- Professor Ying Diao ([http://diao.scs.illinois.edu/Diao\\_Lab/](http://diao.scs.illinois.edu/Diao_Lab/)), University of Illinois at Urbana-Champaign
- Professor Charles M. Schroeder (<https://schroeder.scs.illinois.edu/>), University of Illinois at Urbana-Champaign
- Professor Huimin Zhao (<http://faculty.scs.illinois.edu/~zhaogrp/>), University of Illinois at Urbana-Champaign

## TECHNICAL STRENGTH

- **Technical skills**
  - Expertized in all-atom and coarse grained molecular dynamics (MD), Monte Carlo simulations, biased sampling methods including metadynamics, umbrella sampling and replica-exchange MD (relevant coursework: Chem 576 *Computational Chemical Biology*).
  - Experienced in statistical free energy methods, including free energy perturbation, thermodynamic integration, weighted histogram analysis method (WHAM), multistate Bennett acceptance ratio (MBAR), and alchemical free energy calculations.
  - Expertized in stochastic modeling of time series data, particularly in Markov modeling of complex protein dynamics from large-scale molecular simulations..
  - Experienced in high-performance computing, parallel programming and computing in multi-core CPU and GPU. (relevant coursework: CS 483 *Applied Parallel Programming*)
  - Experienced in data mining, statistical modeling, machine learning and deep learning, as well as their applications for efficient sampling in molecular simulations and small molecule discovery (relevant coursework: CS 483 *Applied Parallel Programming, Machine Learning, Deep Learning Specialization*).
  - Familiar with theory and tools of bioinformatics and cheminformatics (relevant coursework: CS 466 *Introduction to Bioinformatics*).
  - Familiar with algorithms and data structures, and exposure to web development and scientific visualization (relevant coursework: *Algorithms Specialization, CSE 527 Scientific Visualization*).
- **Programming**
  - Experienced in Python, C/C++, shell scripting.
  - Familiar with GPU programming, CUDA and OpenACC; working knowledge of OpenMP.
  - Exposure to SQL, MATLAB, JavaScript, HTML.
- **software**

- **Modeling:** Amber, OpenMM, NAMD, Gromacs, VASP, Schrodinger, AutoDock, Rosetta, Chimera
- **Data mining:** NumPy, SciPy, Pandas, MDTraj, MSMBuilder, Osprey
- **Machine learning:** Scikit-learn, TensorFlow, Keras, MXNet, DeepChem
- **Visualization:** PyMOL, VMD, Matplotlib, D3.js, Origin
- **Others:** Git,  $\text{\LaTeX}$ , Microsoft office, MATLAB, Octave

## CERTIFICATES

- Completion of Deep Learning, a 5-course specialization (including computer vision and natural language processing) by deeplearning.ai on Coursera, 2019.
- Completion of Machine Learning by Stanford University on Coursera, 2019.
- Completion of Algorithms, a 4-course specialization by Stanford University on Coursera, 2019.

## 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.