

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
 - Advisors: Professor Lingti Kong (<https://nes.sjtu.edu.cn/english.htm>), Professor Cheng Zhong
- **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 developments 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 23rd 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.[†], Deb A.[†], **Zhao C.**, Moffett A.S. and Shukla D. (2019). Molecular dynamics simulations reveal the perception of brassinosteroids by the plant receptor BRI1. In review. (†: **co-first** author, same below)
2. Cuculis L.[†], **Zhao C.**[†], Abil Z., Zhao H., Shukla D. and Schroeder C.M. (2019). Divalent Cations Promote TALE DNA-binding Specificity. In review.
3. **Zhao C.** and Shukla D. (2019). Molecular Basis of the Activation and Dissociation of Dimeric PYL2 Receptor in Abscissic Acid Signaling. In review. (bioRxiv DOI: 10.1101/721761)
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.[†], **Zhao C.**[†] and Shukla D. (2019). Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. **Structure**, 27, 692-702.e3.
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 Shuka D. (2019) Quantitative Characterization of Protein-Ligand and Protein-Protein Binding Processes Involved in Plant Hormone Signaling. AIChE Annual Meeting, Orlando, FL. (accepted)
2. **Zhao C.** and Shuka D. (2019). Molecular Basis and Engineering of Plant Drought Resistance Signaling. GLCACS 23rd Annual Conference, Chicago, IL.
3. **Zhao C.** and Shuka 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 Shuka 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 Shuka D. (2018). Dewetting controls plant hormone perception and initiation of drought resistance signaling. 17th 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. 253rd 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 Shuka D. (2019) Towards Rational Design of Chemical Modulators to Improve Plant Drought Tolerance. AIChE Annual Meeting, Orlando, FL. (accepted)
2. **Zhao C.** and Shukla D. (2018). Complex dynamics of hormone perception and receptor activation in plant drought resistance signaling. 256th 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. 253rd 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. 61st 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[†], Zhao[†] and Shukla, Structure, 2019; Zhao and Shukla, 2019 (in review); Aldukhi[†] and Deb[†] *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** 2019/02-Present

- 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[†] and Zhao[†] *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, incoming M.S. student at King Abdullah University of Science and Technology
- Aik Rui Tan, MatSE'19, incoming 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 Z. Anorg. Allg. Chem.
- Journal co-reviewer for J. Chem. Phys., J. Phys. Chem. B., J. Chem. Inf. Model.

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.

• Softwares

- **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, L^AT_EX, 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.