Curriculum Vitae: Chuankai Zhao

CONTACT INFORMATION

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EDUCATION

- **Ph.D.**, Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign   2020
  - Concentration Program: Computational Science & Engineering
  - Advisor: Prof. Diwakar Shukla
- **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: Prof. Lingti Kong
- **Summer Program**, Entrepreneurship, National University of Singapore   2014

HONORS & AWARDS

- 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. **Zhao C.** and Shukla D. (2019). Molecular Basis of the Activation and Dissociation of Dimeric PYL2 Receptor in Abscisic Acid Signaling. In review.
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. (* denotes **co-first** author)
3. 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**, in press, DOI: 10.1021/acsami.9b02923.
4. Shukla S.*, **Zhao C.*** and Shukla D. (2019). Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. **Structure**, 27, 692-702.e3. (* denotes **co-first** author)

5. **Zhao C.** and Shukla D. (2018). SAXS-guided Enhanced Unbiased Sampling for Structure Determination of Proteins and Complexes. **Scientific Reports**, 8, 17748.

6. 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.)

7. 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.** and Diwakar Shukla. (2019). Molecular Basis and Engineering of Plant Drought Resistance Signaling. GLCACS 23rd Annual Conference, Chicago, IL.

2. **Zhao C.** and Diwakar Shukla. (2019). Molecular Basis and Engineering of Plant Drought Resistance Signaling. Science & Spirits Lightning Talks, University of Illinois, Urbana, IL. (invited)

3. **Zhao C.** and Diwakar Shukla. (2018). Structural, dynamic and energetic basis of plant hormone signal transduction. Photosynthesis Research Unit Seminar, University of Illinois, Urbana, IL.

4. **Zhao C.** and Diwakar Shukla. (2018). Dewetting controls plant hormone perception and initiation of drought resistance signaling. 17th Annual Gradaute Research Symposium, Chemical and Biomolecular Engineering at Illinois, Urbana, IL.

5. 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.

6. 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. 256th 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. 253rd 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. 61st 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.

RESEARCH EXPERIENCE

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

- **Revealing 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 publication: Shukla* and Zhao* *et al.* Structure, 2019; Zhao and Shukla, 2019 (in review).

- **Characterizing the Plant Hormone Binding Effects on Protein-Protein Association (ongoing)**
  - 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).

- **Agrochemical Discovery using Machine Learning (ongoing)**
  - Employed the agrochemical datasets from ChemBL and trained deep neural network (DNN) and classical machine learning models to predict agrochemical-likeness of small molecules.
  - Trained DNN and classical models to classify subtypes of agrochemicals and define agrochemical space.

- **Experimental-guided Sampling Method for Large-scale Molecular Simulations**
  - Developed a Markov chain adaptive sampling algorithm for molecular simulation with sparse computational and experimental data incorporated, leading to >50% reduction in computation time in sampling protein folding and protein-protein association processes.
  - Demonstrated application in integrative modeling of near-native 3D structures of proteins and complexes.
  - Related publication: Zhao and Shukla. Sci. Rep., 2018.

- **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 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 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 publication: Mohammadi *et al.* Nat. Commun., 2017; Mohammadi *et al.* 2019 (in review).

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.
  - Won the Excellent Project Award of Undergraduate Innovation Program.

– 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:

- 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

- Reviewer for Z. Anorg. Allg. Chem.
- 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, particularly in Markov modeling of complex protein dynamics from large-scale molecular simulations..
  - Experienced in high performance computing, data analysis, statistical modeling and data visualization (relevant coursework: CS 483 *Applied Parallel Programming*, CSE 527 *Scientific Visualization*).
  - Familiar with machine learning and deep learning algorithms as well as their applications in molecular simulations and drug discovery. (relevant coursework: *Machine Learning* (Coursera), *Deep Learning Specialization* (Coursera))
  - 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 visualization (relevant coursework: CSE 527 *Scientific Visualization*).
- **Programming**
  - Experienced in Python, C/C++, shell scripting.
  - Familiar with GPU programming, CUDA and OpenACC; working knowledge of OpenMP (relevant coursework: CS 483 *Applied Parallel Programming*).
  - Exposure to SQL, MATLAB, JavaScript, HTML (relevant coursework: CSE 527 *Scientific Visualization*).
- **Softwares**
  - **Modeling**: Amber, OpenMM, NAMD, Gromacs, VASP, Schrodinger, AutoDock, Rosetta, Chimera
  - **Data analysis**: NumPy, SciPy, Pandas, MDTraj, MSMBuilder, Osprey
  - **Machine learning**: Scikit-learn, TensorFlow, Keras, MXNet, DeepChem

    – **Visualization**: PyMOL, VMD, Matplotlib, D3.js, Origin

    – **Others**: Git, LaTeX, Microsoft office, MATLAB, Octave

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.