Chuankai Zhao

CONTACT INFORMATION

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EDUCATION

Ph.D., Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign   May 2020 (expected)
- Concentration: Computational Science & Engineering
- Advisor: Professor 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: *Ab initio* study of the ideal tensile and shear strength of B2 CuZr
- Advisors: Professor Lingti Kong and Professor Cheng Zhong

HONORS & AWARDS

- 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 Charitable 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. Mohammadi E., **Zhao C.**, Zhang F., Qu G., Jung S.-H., Lee J.-K., Shukla D. and Diao Y. (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.**, 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. **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.**, Deng Y., Hu W. and Zhong C. (2015). Fabrication of Platinum Sub-monolayer 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 signaling. 17th Annual Gradaute 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. 253rd 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. 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**
  - Performed large-scale molecular dynamics and Monte Carlo simulations on petascale supercomputer to unravel complete perception mechanisms of 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.
  - Related publication: Shukla* and Zhao* *et al.* Structure, 2019.

- **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 and complex structures.

  – 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 quantitatively characterize TALE-DNA binding free energy changes in various salt solutions, and unraveled molecular origins of divalent cation effects.

  – Related publications: Cuculis* and Zhao* *et al.* Angew. Chem. Int. Ed., 2019 (under 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 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.* J. Am. Chem. Soc., 2019 (under review).

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.

  – 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:

- Aik Rui Tan, MatSE'19, currently applying for graduate school   2018/05-Present

- Moen Meigooni, ChBE'17, 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 (relevant coursework: Chem 576 *Computational Chemical Biology*).
  - 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 (relevant coursework: CSE 527 *Scientific 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 (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, SQL.
  - Familiar with GPU programming, CUDA and OpenACC (relevant coursework: CS 483 *Applied Parallel Programming*).
  - 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.