Jiangyan Feng

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Education

Ph.D., Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign 2021
Concentration: Computational Science & Engineering
M.S., Chemical & Biomolecular Engineering, University of Illinois at Urbana-Champaign 2019
B.S., Chemical Engineering, Tianjin University, China   2016
Overseas Study, Western University, Canada   2016

Publications

10. Chen R., **Feng J.**, ..., Shukla D., & Su X. (2020). Tunable Metallopolymer Charge Transfer Interactions for Electrochemical Metal Ion Capture and Recovery. (manuscript in preparation)

9. **Feng J.** & Shukla D. (2020). How Antiporters Exchange Substates Across the Cell Membrane? An Atomic-level Description of the Complete Exchange Cycle. (manuscript in preparation)

8. Selvam B. *, **Feng J.***, & Shukla D. (2020). Atomistic Insights into Dual Affinity Mechanism of NRT1.1. (submitted) (* Equal contribution)

7. **Feng J.** & Shukla D. (2020). FingerprintContacts: Predicting Protein Alternative Conformations from Coevolution. J. Phys. Chem. B.

6. **Feng J.***, Chen J.*, Selvam B. *, & Shukla D. (2019). Computational Microscopy: Revealing Molecular Mechanisms in Plants using Molecular Dynamics Simulations. Plant Cell. 31 (12). (* Equal contribution)

5. Chen Q.*, **Feng J.***, Mittal S., & Shukla D. (2018). Automatic Feature Selection in Markov State Models using Genetic Algorithm. J. Comput. Sci. Educ. 9 (2), 14-22. (* Equal contribution)

4. **Feng J.** & Shukla D. (2018). Characterizing Conformational Dynamics of Proteins using Evolutionary Couplings. J. Phys. Chem. B. 122 (3), 1017-1025.

3. **Feng J.**, Oyeneye O., Xu W., & Charpentier P. (2018). In-Situ NMR Measurement of Reactivity Ratios for Copolymerization of Methyl Methacrylate and Diallyl Dimethylammonium Chloride. Ind. Eng. Chem. Res. 57 (46), 15654-15662.

2. Wang S., **Feng J.**, Xie Y., Tian Z., Peng D., Wu H., & Jiang Z. (2016). Constructing Asymmetric Membranes via Surface Segregation for Efficient Carbon Capture. J. Membr. Sci. 500, 25-32.

1. Wang S., Tian Z., **Feng J.**, ..., & Jiang Z. (2015). Enhanced CO_2 Separation Properties by Incorporating Poly (ethylene glycol)-containing Polymeric Submicrospheres into Polyimide Membrane. J. Membr. Sci. 473, 310-317.

Selected Honors & Awards

13. **Second Prize Oral Presentation**, Annual ChBE Graduate Research Symposium, University of Illinois, USA   2019

12. **Harry G. Drickamer Graduate Research Fellowship**, University of Illinois, USA 2019-2020

11. **Chia-chen Chu Fellowship**, University of Illinois, USA   2019, 2018

10. **Area 53 International Speech Contest Second Place**, Toastmasters International, USA 2019

9. **Hanratty Travel Award**, University of Illinois, USA   2019

8. **First Prize Poster Presentation**, Annual ChBE Graduate Research Symposium, University of Illinois, USA   2018

7. **Third Prize**, Mathematical Contest in Modeling, USA   2015

6. **Second Prize**, Academic Science and Technology Competition, China   2015

5. **Overseas Study Scholarship (10 students selected)**, China Scholarship Council, China 2015

4. **Tianjin Municipal People's Scholarship (top 3%)**, China   2015

3. **Awarded Municipal Funding**, National Innovative Training Program, China   2014

2. **Second Prize**, National Mathematical Contest in Modeling, China   2014

1. **Academic Excellence Scholarships (top 5%)**, Tianjin University, China   2014, 2013

Projects: Computational Biology and Machine Learning

Machine Learning for Protein Dynamics Prediction
o Developed a machine learning method for predicting alternative protein conformations through combination of agglomerative clustering and bioinformatics.
o Performed statistical analysis (direct coupling analysis) to extract evolutionary couplings from multiple sequence alignment.
o Related publication: **Feng J.** & Shukla D. (2020). FingerprintContacts: Predicting Protein Alternative Conformations from Coevolution. J. Phys. Chem. B. (in press)
Feng J. & Shukla D. (2018). Characterizing Conformational Dynamics of Proteins using Evolutionary Couplings. J. Phys. Chem. B. 122 (3), 1017-1025.

Automatic Feature Selection for Dimensionality Reduction
o Developed a genetic algorithm based technique to optimize feature selection for dimensionality reduction.
o Related publication: Chen Q.*, **Feng J.***, Mittal S., & Shukla D. (2018). Automatic Feature Selection in Markov State Models using Genetic Algorithm. J. Comput. Sci. Educ. 9 (2), 14-22.

Molecular Dynamics Simulations of Nutrient Transport in Plants (ongoing)
o Performed large-scale all-atom molecular dynamics simulations on petascale supercomputer to unravel the molecular mechanisms of four different transporters.
o Constructed Markov state models to analyze time series simulation data and quantitatively characterized high-dimensional long timescale dynamics, thermodynamics, and kinetics of plant and bacterial transporters.
o Employed genetic algorithm and dimensionality reduction techniques in feature search and selection, and utilized variational cross-validation to optimize parameters for Markov model constructions.
o Related publication: Chen R., **Feng J.**, ..., Shukla D., & Su X. (2020). Tunable Metallopolymer Charge Transfer Interactions for Electrochemical Metal Ion Capture and Recovery. (manuscript in preparation)
Feng J. & Shukla D. (2020). How Antiporters Exchange Substates Across the Cell Membrane? An Atomic-level Description of the Complete Exchange Cycle. (manuscript in preparation)
Selvam B. *, **Feng J.***, & Shukla D. (2020). Atomistic Insights into Dual Affinity Mechanism of NRT1.1. (submitted)
Feng J.*, Chen J.*, Selvam B. *, & Shukla D. (2019). Computational Microscopy: Revealing Molecular Mechanisms in Plants using Molecular Dynamics Simulations. Plant Cell. 31 (12).