


# Jiangyan Feng | Ph.D. Candidate

 Website

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 Github

 Google Scholar

 LinkedIn

## Summary

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- o Forward-thinking computational biologist with 3+ years of experience in developing and using **atomistic simulation, machine learning, and data science approaches** for understanding complex biological processes, leading to **6 publications**.
- o Excellent science communicator, both oral and written, leading to **multiple oral competition awards**.
- o Self-motivated individual with easy-integration in a multicultural environment and proven ability to rapidly learn new problem domains by winning **multiple scientific competition awards**.

## Skills

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### Technical Skills

- o Expertized in all-atom molecular dynamics simulations, biased sampling methods including metadynamics and umbrella sampling.
- o Expertized in stochastic modeling of time series, particularly in Markov modeling of complex protein dynamics from large-scale molecular simulations.
- o Experienced in statistical analysis, such as direct coupling analysis and weighted histogram analysis method (WHAM).
- o Experienced in high-performance computing, large-scale data analysis and modeling, and scientific visualization.
- o Familiar with data mining, machine learning, and deep learning algorithms, and their applications in molecular simulations and protein dynamics.
- o Familiar with theory and tools of bioinformatics.

### Programming

- o Experienced in Python, C/C++, Shell scripting
- o Familiar with GPU programming, CUDA, MySQL, Java
- o Exposure to MATLAB

### Softwares

- o Molecular modeling: Amber, Gromacs, OpenMM, NAMD, Rosetta, Schrödinger's Maestro
- o Data analysis: Jupyter, NumPy, SciPy, Pandas, MDTraj, MSMBuilder, Osprey
- o Machine learning: Scikit-learn, TensorFlow, Keras, DeepChem
- o Visualization: PyMOL, VMD, Matplotlib, Origin
- o Others: Git, LATEX, Microsoft Office, Octave

## Projects: Computational Biology, Molecular Modeling, Machine Learning

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### Machine Learning for Protein Dynamics Prediction (ongoing)

- 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. (2018)**. Characterizing Conformational Dynamics of Proteins using Evolutionary Couplings. J. Phys. Chem. B. 122 (3), 1017-1025.  
**Feng J. & Shukla D. (2019)**. FingerprintContacts: Predicting Protein Alternative Conformations from Coevolution. J. Phys. Chem. B. (submitted)

### 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. (\* Equal contribution)

#### **Pattern Discovery from DNA Sequences**

- o Developed a "motif finding" algorithm to discover patterns in DNA sequences.
- o Codes are available at [https://github.com/JiangyanFeng-PhD/Motif\\_Finder](https://github.com/JiangyanFeng-PhD/Motif_Finder).

#### **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 3 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: **Feng J. \***, Chen J. \*, Selvam B. \* & Shukla D. (2019). Computational Microscope: Revealing Molecular Mechanisms in Plants Using MD Simulations. Plant Cell.

## **Education**

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<b>Ph.D.</b> , Chemical & Biomolecular Engineering, University of Illinois, GPA: 3.78/4.00	2021
<b>Concentration: Computational Science &amp; Engineering</b> , GPA: 4.00/4.00	
<b>M.S.</b> , Chemical & Biomolecular Engineering, University of Illinois	2019
<b>B.S.</b> , Chemical Engineering, Tianjin University, China	2016, GPA: 3.83/4.00
<b>Overseas Study</b> , Western University, Canada	2016

## **Publications**

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1. **Feng J.** & Shukla D. (2019). FingerprintContacts: Predicting Protein Alternative Conformations from Coevolution. J. Phys. Chem. B. (submitted)
2. **Feng J. \***, Chen J. \*, Selvam B. \* & Shukla D. (2019). Computational Microscopy: Revealing Molecular Mechanisms in Plants using Molecular Dynamics Simulations. The Plant Cell. (\* Equal contribution)
3. 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.
5. **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.
6. 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.
7. Wang S., Tian Z., **Feng J.**, ... & Jiang Z. (2015). Enhanced CO<sub>2</sub> Separation Properties by Incorporating Poly (ethylene glycol)-containing Polymeric Submicrospheres into Polyimide Membrane. J. Membr. Sci. 473, 310-317.

## **Selected Honors & Awards**

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1. **Harry G. Drickamer Graduate Research Fellowship**, University of Illinois, USA 2019-2020
2. **Area 53 International Speech Contest Second Place**, Toastmasters International, USA 2019
3. **First Prize Poster Presentation**, University of Illinois at Urbana-Champaign, USA 2018
4. **Third Prize**, Mathematical Contest in Modeling, USA 2015
5. **Second Prize**, National Mathematical Contest in Modeling, China 2014