Yinhao Jia

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PROFESSIONAL SUMMARY

PhD researcher specializing in Molecular Dynamics simulations of soft materials, particularly proteins and polymers. Experienced in analyzing material properties and microscopic behavior through computational modeling. Strong skills in data analysis, problem-solving, and collaboration, with a commitment to advancing therapeutic research.

EDUCATION

University of Florida, Gainesville, FL, USA
Doctor of Philosophy in Chemical Engineering | GPA:3.97/4 — Expected December 2025
Master of Science in Chemical Engineering | GPA: 3.95/4 — May 2022

Zhejiang University of Technology, Hangzhou, CHN
Bachelor of Engineering in Energy Chemical Engineering | GPA: 3.66/5 — June 2020

TECHNICAL SKILLS

- Programming language: Python, Bash
- Molecular Dynamics Simulation Software: GROMACS, LAMMPS, PLUMED
- Visualization & Analysis Tools: VMD, PyMOL, Matplotlib, Pandas

RESEARCH EXPERIENCE

Graduate Research Assistant — February 2021 – Present
Sampath Research Group, Gainesville, FL, USA

- Led the group's protein-related projects, applying various simulation techniques to address challenges such as protein unfolding, protein-protein interactions, and protein-polymer interactions.
- Performed molecular dynamics simulations under varying conditions, uncovering novel protein unfolding pathways under these conditions, suggesting necessity of suitable method for stability enhancement.
- Leveraged well-tempered Metadynamics to investigate protein-protein interactions, elucidating agglomerate mechanism, validated experimental findings and strengthened collaborative research outcomes.
- Simulated uniaxial deformation of silk fibroin to uncover microscopic mechanisms in crystalline regions, enhancing understanding of mechanical properties and guiding the design of more resilient silk fibroin scaffolds.
- Designed an automated workflow for protein/polymer complex simulations, accelerating data acquisition, which streamlined the design process for innovative polymer materials.

Undergraduate Research Assistant — January 2019 – June 2019
Hanfeng Lu Research Group, Hangzhou, CHN

- Conceptualized and developed a cutting-edge Oil Spill Emergency Response Platform tailored for offshore oil facilities, focusing on rapid and effective containment and mitigation.
- Proficiently utilized AutoCAD and SolidWorks to design the primary structure of the facility, ensuring precision and adherence to safety standards.
- Drove intellectual property efforts by composing patent mapping and application documents, resulting in successful acceptance as both a patent for invention and a utility model.

Undergraduate Research Assistant — September 2017 – June 2020
Qunfeng Zhang Research Group, Hangzhou, CHN

- Led research on the synthesis of doped active carbon-loaded Palladium (Pd) catalysts, focusing on nitrogen (N) and sulfur (S) sources with varying valence states, and investigating their catalytic performance in the selective hydrogenation of o-CNB to o-CAN, achieving 99% towards selectivity to o-CAN.
- Applied a comprehensive suite of advanced characterization techniques, including X-ray Photoelectron Spectroscopy (XPS), Brunauer-Emmett-Teller (BET) surface area analysis, Scanning Electron Microscopy (SEM), and X-ray Fluorescence (XRF), to evaluate the structural, chemical, and catalytic properties of the synthesized materials, elucidate the mechanism of excellent selectivity.

TEACHING & MENTORING EXPERIENCE

Teaching Assistant

ECH4714, Chemical Process Safety, University of Florida

- Developed course materials integrating CAMEO software, bridging the gap between theory and practice, and enhancing students' ability to apply textbook knowledge to real-world safety scenarios.
- Designed exam questions that effectively transitioned the course from open-book to closed-book assessments, challenging students to strengthen their retention and application of core safety concepts.

Mentor

Summer Undergraduate Research at Florida, University of Florida

- Mentored two undergraduate students in summer research projects on protein behavior under denaturation conditions, guiding them through experimental design and data analysis.
- Achieved one peer-reviewed publication and students present their findings at the AIChE annual student conference, where one student secured 3rd place in the Computing and Process Control division.

PUBLICATION

- **Jia, Y**., Fernandez, A., & Sampath, J. (2023). PEGylation of insulin and lysozyme to stabilize against thermal denaturation: A molecular dynamics simulation study. *The Journal of Physical Chemistry B*, *127*(31), 6856–6866. https://doi.org/10.1021/acs.jpcb.3c01289
- Aikman, E. L., Rao, A. P., **Jia, Y**., Fussell, E. E., Trumbull, K. E., Sampath, J., & Stoppel, W. L. (2024). Impact of crystalline domains on long-term stability and mechanical performance of anisotropic silk fibroin sponges. *Journal of Biomedical Materials Research Part A*, *112*(9), 1451-1471. https://doi.org/10.1002/jbm.a.37703
- Shin, J., **Jia, Y.**, Sampath, J., & Jang, Y. (2024). Phase transition of recombinant fusion protein assemblies in macromolecularly crowded conditions. *Materials Advances*, *5*(10), 4200–4208. https://doi.org/10.1039/d3ma01012k
- **Jia, Y.,** Horvath, K., Jain, P. K., & Sampath, J. Exploring the Thermostability of CRISPR–Cas12b using Molecular Dynamics Simulations. Under review. https://doi.org/10.48550/arXiv.2408.11149
- **Jia, Y.,** Cocker, C., & Sampath, J. Insights into Protein Unfolding under pH, Temperature, and Shear using Molecular Dynamics Simulations. Under review. https://doi.org/10.48550/arXiv.2408.11147

HONORS & AWARDS

- Peer Mentoring Award, Department of Chemical Engineering, University of Florida (2024)
- Graduate Student Council Travel Grant, Graduate Student Council, University of Florida (2024)
- Chemical Engineering Excellence Award, Department of Chemical Engineering, University of Florida (2022)
- Third Prize, National Energy Conservation and Emission Reduction and Science and Technology Competition (2019)
- First Prize, Energy Conservation and Emission Reduction and Science and Technology Competition of ZJUT (2019)
- Second Prize, Zhejiang College Students Physics (Theory) Competition (2018)