Yu Zhu

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EDUCATION

University of Memphis Memphis, TN
Doctor of Philosophy in Applied Physics (GPA: 3.7/4.0) *Aug 2018 – July 2023*

- Thesis (*Master of Computational Physics*): Ring Polymers as a Model for Cellular Organization
- Dissertation: Lipid Membrane-Mediated Interactions and Self-Assembly of Janus Nanoparticles

Bachelor of Science in Physics (GPA: 3.9/4.0) *Aug 2014 – May 2018*

Georgia Institute of Technology Atlanta, GA
Master of Science in Computer Science (GPA: 3.7/4.0) *Jan 2022 – May 2025*

SKILLS

Languages and Tools: C/C++, Python, bash script, SQL, GROMACS, Amber, PyMOL, MDAnalysis, TensorFlow, PyTorch, Git, Vim, slurm, VMD, xmgrace, Latex
Related Courses: Probability/Statistics, Differential Equations, Machine Learning for Trading, Computer Networks, Software Dev Process, Machine Learning, SQL for Data Science, Mechanical Behavior Of Materials, Quantum Mechanics, Soft Matter/Biological Physics, Polymer Physics, Algorithms/Problem Solving, Methods/Computational Physics, Statistical Mechanics, Electrodynamics, Materials Physics
Miscellaneous Technologies: Time series analysis, High-Performance Computing, Monte Carlo, Molecular dynamics, data visualization, mathematical modeling, Random forests, Reinforcement learning, lipid membranes, polymers, self-assembly, collective behavior, free energy calculations, multi-scale modeling

WORK EXPERIENCE

Position: Postdoctoral Associate August 2023 - Current
Project: Multi-Scale modeling of lipid nanoparticles and proteins *Eli Lilly & Purdue University*

- Developed a progressive coarse-graining tool for mapping all-atom protein models into highly coarse grained protein models using essential dynamics and fixed length methods, and a neural network model to back mapping coarse-grain proteins into all-atom models.
- Developed a coarse-grainning tool to construct and parameterize lipid nanoparticles using all-atom simulations.

Position: Research Assistant August 2019 - July 2023
Project: Self-assembly of janus nanoparticles on lipids membranes *University of Memphis*

- Developed a C++ template to create a model of soft, controllable tessellated spherical nanoparticle, whcih was integrated with our coarse grained lipid membrane system. Wrote a large number of analysing scripts, using C++, python, and bash, including the Voronoi diagram both in two and three dimensions, radial distribution function, various types of order parameters, Lindemann measure, auto-correlation functions, diffusion, free energies, etc.
- Performed a comprehensive study of the spatial arrangement of two Janus nanoparticles on the outer or inner side of lipid vesicles by using molecular dynamics method, in conjunction with the calculation of free energy by using weighted histogram analysis method.
- Performed extensive molecular dynamics simulations to show that highly ordered self-assemblies of NPs can be mediated by their adhesion to lipid vesicles. Specific geometries of the nanoassemble could be achieved, including several deltahedra and three Platonic solids, corresponding to the tetrahedron, octahedron, and icosahedron.
- Performed large scale simulations of Janus nanoparticles adhere to the periodic planar lipid membranes to show that the nanoparticles self assembly into hexagonal lattice with quasi-long-range order and a hexatic phase at intermediate densities. I also showed that the melting of nanoparticles from crystal phase to liquid phase agree with KTHNY theory by characterizing Lindemann parameter, bond-order correlation parameter, etc.
- Performed molecular dynamics simulation of Janus nanoparticles on tubular membranes and showed that the nanoparticles can self-assemble into helical nanoassemblies with variable pitch.
- Closely collaborated with other students to explore the modes of adhesion of spherocylindrical nanoparticles to tensionless lipid membranes, membrane-mediated dimerization of spherocylindrical nanoparticles, and the self-assembly of Janus spherocylindrical nanoparticles on lipid vesicles.

Project: Ring polymers as a model for cellular organization *University of Memphis*

- Developed a Metropolis Monte Carlo code and an effcient molecular dynamics software with C++, and OpenMP for the study of the conformational behavior of disjoint ring polymers as a function of their areal density, and degree of flexibility on the substrate.
- Based on the model of ring polymers, developed analysis tools to explore the collective motion of self-propelled particles(cells), and the vorticity Reversals of self-propelled particles (cells) on Circularly Patterned Substrates.

Position: Teacher Assistant August. 2018 – August. 2020

- Taught undergraduate level Physics Lab($I - III$), set up experiments, Proctored tests, and graded coursework.

PUBLICATIONS

- **Zhu, Y.**, Kumar, P. B. S., & Laradji, M. (2021). Conformational behavior and self-assembly of disjoint semi-flexible ring polymers adsorbed on solid substrates. *Soft Matter*, 17(21), 5427–5435.
- Wen, H., **Zhu, Y.**, Peng, C., Kumar, P. B. S., & Laradji, M. (2022). Collective motion of cells modeled as ring polymers. *Soft Matter*, 18(6), 1228–1238.
- **Zhu, Y**., Sharma, A., Spangler, E. J.,& Laradji, M. (2022). Modes of adhesion of two Janus nanoparticles on the outer or inner side of lipid vesicles. *Soft Matter*, 18(25), 4689–4698.
- Sharma, A., **Zhu, Y.**, Spangler, E. J., & Laradji, M. (2022). Modes of adhesion of spherocylindrical nanoparticles to tensionless lipid bilayers. *The Journal of Chemical Physics*, 156(23), 234901.
- Wen, H., **Zhu, Y.**, Peng, C., Kumar, P. B. S., & Laradji, M. (2023). Collective vortical motion and vorticity reversals of self-propelled particles on circularly patterned substrates. *Physical Review E*, 102(7)
- Sharma, A., **Zhu, Y.**, Spangler, E. J., Carrillo, Y. J., & Laradji, M. (2023). Membrane-Mediated Dimerization of Spherocylindrical Nanoparticles. *Soft matter*, 19(8), 1499-1512.
- **Zhu, Y.**, Sharma, A., Spangler, E. J., Carrillo, Y. J., Kumar, P. B. S., & Laradji, M. (2023). Lipid Vesicles Induced Ordered Nanoassemblies of Janus Nanoparticles. *Soft matter*, 12(19) 2204-2213.
- **Zhu, Y.**, Sharma, A., Spangler, E. J., & Laradji, M. (2023). Non-Close-Packed Hexagonal Self-Assembly of Janus Nanoparticles on Planar Membranes, *Soft Matter*, 39(19), 7591-7601.
- **Zhu, Y.**, Zhao, X.,Xiang,C., Liu, Xianshi, & Li, J (2024). Evaluation of Essential Dynamics and Fixed-Length Coarse Graining for Multidomain Proteins, *J. Phys. Chem. B*, 128(21), 5147–5156.
- Sharma, A.,**Zhu, Y.**, Spangler, E. J., Hoang, T. B., & Laradji, M. (2024). Highly Ordered Nanoassemblies of Janus Spherocylindrical Nanoparticles Adhering to Lipid Vesicles, *ACS Nano* 18(20), 12957–12969.
- **Zhu, Y.** & Laradji, M. Star-Like Self-Assemblies of Spherical Nanoparticles Inside Lipid Vesicles, *Under preparation*
- **Zhu, Y.**,& Li, J. Recovery of Atomistic Protein Structures from Low-Resolution Models using Machine Learning, *Under peraparation*

PRESENTATIONS

- **Zhu, Y.**, Kumar, P. B. S., & Laradji, M. "Shapes and Spatial Organization of Self-Avoiding Semiflexible Ring Polymers on Solid Substrates", Poster at APS march meeting, March 2021
- **Zhu, Y.**, Spangler, E. J., & Laradji, M. "Assembly of Janus Nanoparticles on Lipid Vesicles", Poster at APS march meeting, Chicago, IL, March 2022
- **Zhu, Y.**, Sharma,A, Spangler, E. J., & Laradji, M. "Lipid Vesicles Induced Ordered Nanoassemblies of Janus Nanoparticles", Talk at APS march meeting, Las Vegas, NV, March 2023
- Sharma, A, **Zhu, Y.**, Spangler, E. J., & Laradji, M. "Adhesion and Dimerization of Spherocylindrical Nanoparticles on Tensionless Lipid Bilayers", Talk at APS march meeting, Las Vegas, NV, March 2023
- **Zhu, Y.**, Sharma, A, Spangler, E. J., & Laradji, M. "Non-Close-Packed Hexagonal Self-Assembly of Janus Nanoparticles on Planar Membranes", Talk at ACS Colloid and Surface Science Symposium, Raleigh, NC,June 2023
- **Zhu, Y.**, Sharma, A, Spangler, E. J., & Laradji, M. "Aster Self-Assemblies of Spherical Nanoparticles Adhering to the Inner Side of Lipid Vesicles", Poster at ACS Colloid and Surface Science Symposium, Raleigh, NC, June 2023
- Sharma, A., **Zhu, Y**, Spangler, E. J., & Laradji, M. "Lipid Vesicles Induced Ordered Nano-assemblies of Janus Spherocylindrical Nanoparticles", Talk at ACS Colloid and Surface Science Symposium, Raleigh, NC, June 2023
- Sharma, A, **Zhu, Y.**, Spangler, E. J., & Laradji, M. "Two-dimensional Nanoassemblies of Spherocylindrical Nanoparticles inside Lipid Vesicles", Poster at APS march meeting, Minneapolis, MN, March 2024
- **Zhu, Y.**, Sharma, A, Spangler, E. J., & Laradji, M. "Liposomes-Induced Nanostar Self-Assemblies of Spherical Nanoparticles", Poster at APS march meeting, Minneapolis, MN, March 2024
- **Zhu, Y.**, Zhao, X, & Li, J. "Systematic investigation of coarse-grained mapping and back mapping for proteins", Talk at ACS Spring meeting, New Orleans, LA, March 2024