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Yuanming Song
Computational Chemist

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EDUCATION

University of California, Irvine *(Advisor: Douglas J. Tobias)* — *Irvine, CA*
Ph. D. Physical Chemistry — **August 2025**
Thesis: *In Silico* Studies and Design of Redox-Responsive Self-Assembling Molecules

University of Redlands *(Advisor: Michael J. Ferracane)* — *Redlands, CA*
B. S. Chemistry (ACS Undergraduate Award in Analytical Chemistry) — **Dec 2018**
Thesis: Synthesis and Characterisation of κ Opioid Receptor (KOR) Antagonists

RESEARCH EXPERIENCE

Junior Research Fellow — **Sep 2025-Present**
Department of Chemistry, University of California, Irvine — *Irvine, CA*

- Designed and executed benchmarking of **LLM**-accelerated **molecular dynamics (MD)** against conventional MD on GLP-1R–Danuglipron complex for fast conformation generation of protein–ligand systems, and downstream free energy–based calculations.
- Developed **agentic workflows** to automate pipeline development, benchmarking, and validation, reducing iteration time for simulation and analysis pipelines.

Graduate Student Researcher (Advisor: Douglas J. Tobias) — **May 2020-August 2025**
Center for Complex and Active Materials (NSF MRSEC)
Department of Chemistry, University of California, Irvine — *Irvine, CA*

- Innovated and automated a high-throughput, physics-based, **AI**-accelerated simulation pipeline for understanding biomolecular active self-assembly, integrating **MD** simulations, **deep learning**, and exponential-family random graph models (**ERGM**)-based intermolecular interaction analysis for ranking candidates.
- Generated and analyzed large-scale simulation datasets to train predictive models, with model-selected compounds currently being validated experimentally.
- Performed **free energy calculations** on biomolecules and small molecules using **umbrella sampling** and **metadynamics** to interpret spectroscopic measurements.
- Parameterized physics-based model multi-conformational Monte Carlo (**mcMC**) and graph-based statistical model Network Hamiltonian Models (**NHM**), based on experimental and **MD** generated datasets and maximum likelihood estimation via Snijders stochastic approximation.
- Coordinated interdisciplinary research with 11 collaborators across 6 groups—leading to 4 publications (2 as first author) and additional manuscripts in preparation.

Research Assistant — **Jun-Aug 2018**
Infinity Innovation Inc. (Peidong Yang Centre) — *Suzhou, China*

- Developed and implemented robust quality control protocols for magnetic beads at an early-stage startup, resolving process standardization challenges to ensure consistent product performance. Product performace were validated using **ELISA**, **Zetasizer**, **SEM**, and **flow cytometry**.

Undergraduate Research Assistant (Advisor: Michael J. Ferracane) — **Jan 2017- Dec 2018**
Department of Chemistry, University of Redlands — *Redlands, CA*

- Screened with free energy calculations and synthesized cyclic tetrapeptide analogs as novel candidates for opioid addiction therapeutics, optimizing reaction conditions to enhance yield and efficacy.
- Purified and characterized peptides using **LC-MS** and **NMR** techniques, providing high-quality compound analysis to support drug development efforts.

PUBLICATIONS

- **Song, Y.** *Active Self-Assembling Peptide Materials Screening and Design using Molecular Dynamics, Deep Learning, and Graph Theory. In preparation, awaiting experimental results.*
- **Song, Y.**; Li, Z.; Mulvey, J.; Freites, J. A.; Patterson, J.; Tobias, D. J. *Cryo-EM Informed Molecular Dynamics Simulations to Investigate the Disulfide Hydrogel Self-Assembly. ChemPhysChem* **2025**, *26*, May.
- **Song, Y.**; Serxho, S.; Freites, J. A.; Guan, Z.; Tobias, D. *Multiscale Molecular Dynamics Simulations of an Active Self-Assembling Material. J. Phys. Chem. B* **2024**, *128*, Jan. 30.

- Urbach, Z. J.; Marrufo, N.; Do, Q. T. H.; Le, J. N.; Wierzbicki, M.; **Song, Y.**; Mustafa, K.; Wang, F.; Egelman, E. H.; Guan, Z.; Tobias, D. J.; Hochbaum, A. I. *Sequence Programmable Order–Disorder Transitions in Supramolecular Assembly of Peptide Nanofibers. J. Am. Chem. Soc.* **2025**, *147*, 24699–24707.
- Mohanam, L.; Umeda, R.; Gu, L.; **Song, Y.**; Tobias, D.; Hochbaum, A.; Wu, R.; Sharifzadeh, S. *Investigating Electron Conductivity Regimes in the Bacterial Cytochrome Wire OmcS. ACS Nano*, *in review.*
- **Song, Y.** *Free Energy Molecular Dynamics Analysis of pH Sensitivity in Coiled-Coil Peptide Secondary Structure.* ChemRxiv, preprint, May 2025, DOI: 10.26434/chemrxiv-2025-2lln2.
- **Song, Y.** *Evaluating SIRAH Force Field for Modeling Spontaneous and Redox-Responsive Peptide Self-Assembly.* ChemRxiv, preprint, May 2025, DOI: 10.26434/chemrxiv-2025-1lthl.
- **Song, Y.** *Synthesis and Characterization of κ Opioid Receptor (KOR) Antagonists.* Undergraduate Thesis, 2018.

AWARDS & HONORS

- **MRSEC JRF Research Award** (2025) - IRG-2, University of California, Irvine

PROFESSIONAL SKILLS

Programming:	Python, C++, R, Linux Shell Scripting (Bash/Zsh), SQL, Tcl/Tk
High-Performance Computing:	Job Scheduling (SLURM, PBS), Parallel Computing, GPU Acceleration
Molecular Dynamics:	Force Fields: CHARMM, SIRAH, MARTINI; Techniques: Umbrella Sampling, Multi-Conformational Monte Carlo (mcMC), Network Hamiltonian, Gaussian-Accelerated MD (GaMD), Replica Exchange MD (REMD), Chemical Graph Theory
Deep Learning:	Preparing data for and training models including Transformer, GraphSAGE, GTN, GNN, MLP in PyTorch
Software & Packages:	Schrodinger, VMD, NAMD, GROMACS, MOE, CGenFF, PyMOL, AlphaFold, Rosetta, RFdiffusion, RDKit, Mnova, VnmrJ, Anton-specific software
Laboratory Techniques:	SPPS, Liquid-Phase Peptide Synthesis, FREP, ELISA with Magnetic Beads, Peptide 3D-Structure Analysis (NMR)
Instrumentation:	LC-MS, GC-MS, HPLC, AA/AES, 1D & 2D NMR, UV-Vis, Flash Chromatography, Zetasizer, SEM, Flow Cytometry

SELECTED PRESENTATIONS

- **Song, Y.** *Redox-Responsive Biomaterials: A Synergistic Approach to Peptide Self-Assembly Using Molecular Dynamics and Experimental Screening.* Presented at *BPS2025*, Feb. 17, 2025.
- **Song, Y.**; Serxho, S.; Freites, J. A.; Guan, Z.; Tobias, D. *Multi-scale Molecular Dynamics Simulations of Active Supramolecular Materials.* Presented at *SoCalTheoChem*, Oct. 14, 2023.
- **Song, Y.**; Ferracane, M. *Synthesis and Characterization of Prolonged κ Opioid Receptor Antagonistic Cyclic Tetrapeptide Analogs.* Presented at *Southern California Conferences for Undergraduate Research (SCCUR)*, Pasadena, CA, Nov. 17, 2018.

LEADERSHIP & MENTORING EXPERIENCE

Mentor for Undergraduate Researchers **Jan 2021-Present**
Center for Complex and Active Materials (NSF MRSEC)
Department of Chemistry, University of California, Irvine *Irvine, CA*

· Mentored four undergraduate students in applying MD simulations to study self-assembling peptides and small molecules, providing hands-on training in simulation techniques and data analysis.
· Developed and delivered comprehensive STEM education and outreach modules for MRSEC initiatives, designing instructional activities and presentations that engaged over 400 high school and undergraduate students.

LANGUAGES

Native:	Chinese (Mandarin), English