Weizhou Wang

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Research Profile

Theoretical chemistry PhD student developing generative and probabilistic sampling methods for molecular simulation, statistical mechanics, and AI for Science. Current work focuses on diffusion/flow-based molecular sampling, path-integral quantum statistics, posterior inference under physical constraints, and reusable generative priors for scientific simulation.

EDUCATION

University of Chicago, Chicago, USA Sep 2024 - Present

- Ph.D. Student, Theoretical Chemistry. Co-advised by Prof. Aaron Dinner (UChicago Chemistry) and Prof. Jonathan Weare (Courant Institute, NYU).
- Neubauer Graduate Fellow

Peking University, Beijing, China Aug 2020 - Jul 2024

- B.S. in Chemistry (GPA 3.72/4.0; Rank: Top 15%)

Honors and Awards

- 2026 Josef Fried Graduate Fellowship
- 2023 Jiu Kun Scholarship, 2023 Academic Excellence Award
- 2022 Chung Yong-hee Scholarship, 2022 Outstanding Scientific Research Award

Technical Skills

Programming / ML: Python, PyTorch, NumPy, SciPy, Git, Linux, SLURM, GPU training

Molecular Simulation: OpenMM, MDTraj, molecular dynamics, path-integral molecular dynamics, enhanced sampling

Methods: diffusion/flow models, MCMC/Gibbs sampling, statistical mechanics, posterior inference.

Relevant Topics: AI for molecular simulation, quantum statistics, rare-event, physics-aware generative model.

Research Experience

Generative Posterior Sampling for Molecular Systems under Physical Contexts| University of Chicago | Graduate Research | Nov 2025 – Present

- Developed **GG-PA**, a training-free framework for composing pretrained molecular generative priors with physical contexts without retraining
- Benchmarked GG-PA on lattice and biomolecular peptide systems, demonstrating context-induced distribution shifts and emergent collective behaviors under changing physical environments.
- Relevant to **inference-time conditioning**, **enhanced sampling**, **physical constraints in generative models** and **molecular simulation across changing chemical environments**.

Quantum Statistics from Classical Simulations via Generative Gibbs Sampling | University of Chicago | Graduate Research | Jan 2025 – Present

- Developed **GG-PI**, a generative sampling framework that learns path-integral single-bead conditional distribution from standard molecular dynamics data, reducing reliance on costly PIMD simulations.
- Enabled transfer across temperatures without retraining by exploiting the fixed-imaginary-interval conditional structure.
- Achieved substantial wall-clock speedup relative to PIMD while maintaining strong accuracy on benchmark systems including Zundel ion, bulk water and para-hydrogen.

Preprints / Manuscripts

Weizhou Wang, Jonathan Weare, Aaron R. Dinner. Composing Diffusion Priors with Explicit Physical Context via Generative Gibbs Sampling. *arXiv: 2605.10642*, (2026).

Weizhou Wang, Xuanxi Zhang, Jonathan Weare, Aaron R. Dinner. Quantum Statistics from Classical Simulations via Generative Gibbs Sampling. *arXiv: 2601.20228*, (2026). Under review.

Publications

Weihao Liang, Sihan Wang, Cong Wang, **Weizhou Wang**, Xinchen She, Chongbin Wang, Jiushu Shao, Jian Liu. An Efficient Integrator Scheme for Sampling the (Quantum) Isobaric-Isothermal Ensemble in (Path Integral) Molecular Dynamics Simulations. *J. Chem. Theory Comput*. **2025**, *21*(13), 6394-6409.