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Wesley
Oliver

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Professional Summary

Fourth year Ph.D. candidate. Computational chemist by training with expertise in machine learning-driven molecular design and simulation. Developed feature engineering approaches for protein property prediction using deep learning architectures. Experience spans molecular dynamics simulations (LAMMPS, GROMACS) to ML models in Python. Published researcher with proven technical communication skills.

Research Experience

Graduate Research Assistant

Princeton University

Princeton, NJ

January 2023-Present

- *Advisor:* Professor Michael Webb
- Create novel “physically-informed” features to improve ML model predictions of protein properties
- Develop ML models using TensorFlow, PyTorch, and scikit-learn to predict protein phase behavior from molecular simulation data
- Regularly employ advanced computational methods including enhanced sampling techniques (ABF, REMD) and free energy calculations (TI, FEP)
- Developed expertise with tools such as LAMMPS and GROMACS to perform high-throughput atomistic and coarse-grained molecular simulations
- Simulated systems of DNA to investigate the incorporation of non-native nucleic acids on DNA structure
- Collaborate with experimentalists to corroborate experimental findings using simulation data
- Conducting an active-learning campaign to explore design tradeoffs in intrinsically disordered proteins
- Use reinforcement learning control over molecular simulations to influence the morphology of sequence-defined materials

Undergraduate Research Assistant

Purdue University

West Lafayette, IN

August 2019-December 2021

- *Advisor:* Professor David Corti
- Conducted computational research on Hamaker constants, a value that quantifies the strength of van der Waals interactions
- Modeled atomic force microscope (AFM) force experiments to investigate the impact of considering repulsive forces on Hamaker constant estimation

Technical Skills

Programming Languages: Python (NumPy, pandas, scikit-learn, MDAnalysis, multiprocessing, Joblib), MATLAB, C

Machine Learning: TensorFlow, PyTorch, reinforcement learning (Q-learning)

Molecular Simulation: LAMMPS, GROMACS, enhanced sampling, free energy calculations, atomistic and coarse-grained MD

Education

Princeton University

Ph.D., Chemical and Biological Engineering

Advisor: Michael Webb, Ph.D.

Princeton, NJ

expected May 2027

Purdue University

B.S., Chemical Engineering

GPA: 4.0/4.0

West Lafayette, IN

December 2021

Industry Experience

Process Research and Development Intern

The J. R. Simplot Company

Caldwell, ID

Summer 2021

- Developed a quantitative methodology to analyze food processing efficiency in seasoning application
- Designed and executed pilot plant scale experiments, leading a team of three research technicians
- Created user-friendly interfaces in Excel and ImageJ that automated the evaluation of experimental results

Facilities Engineering Intern

ExxonMobil

Williston, ND

Summer 2020

- Designed a data collection system to track factors leading to equipment failures in oil field operations
- Applied statistical analysis to historical failure data to optimize maintenance scheduling
- Led an investigation into vapor recovery units using Aspen and MATLAB, creating an economic evaluation tool

Teaching Experience

Course Coordinator & Tutor

Prison Teaching Initiative

Princeton, NJ

September 2023 - Present

- Developed and delivered associate-level mathematics curriculum at Garden State Youth Correctional Facility, coordinating instruction across multiple educators
- Manage a team of tutors conducting weekly tutoring sessions for college students at Northern State Prison
- Volunteered a total of approximately 160 hours teaching and tutoring college students at state correctional facilities

Assistant Instructor

Princeton University

Princeton, NJ

Spring 2024 & 2025

- Two time assistant instructor for CBE 246, Princeton's undergraduate level thermodynamics course
- Created lesson plans, developed practice problems, and taught weekly discussion sections of approximately 25 students
- Graded problem sets and exams and held weekly office hours

Awards & Honors

- 3rd place out of 30+ teams, chemical engineering senior design project

Publications

Jin, J., **Oliver, W.**, Webb, M. A., & Jacobs, W. M. (2025). Predicting heteropolymer phase separation using two-chain contact maps. *The Journal of Chemical Physics*, 163(1), 014102.

Oliver, W., Jacobs, W. M., & Webb, M. A. (2025). When B_2 is not enough: Evaluating simple metrics for predicting phase separation of intrinsically disordered proteins. *The Journal of Physical Chemistry B*, 129(37), 9551–9565.

Vazquez, J. M., **Oliver, W.**, Beaudoin, S. P., & Corti, D. S. (2024). The effects of short-range intermolecular repulsive forces on hamaker constant estimation using atomic force microscopy. *Langmuir*, 40(47), 24808–24819.

Abstracts

Presentations:

Oliver, W., & Webb, M. A. *When B_2 is not enough: Unraveling the limitations of simple metrics for assessing the phase behavior of intrinsically disordered proteins.* ACS Middle Atlantic Regional Meeting, South Orange, NJ. 2025, May.

Oliver, W., & Webb, M. A. *When B_2 is not enough: Unraveling the limitations of simple metrics for assessing the phase behavior of intrinsically disordered proteins.* APS Global Physics Summit, Anaheim, CA. 2025, March.

Posters:

Oliver, W., & Webb, M. A. *Controlled structure formation of sequence-defined materials with reinforcement learning.* ACS Middle Atlantic Regional Meeting, South Orange, NJ. 2025, May.

Oliver, W., & Webb, M. A. *Controlled structure formation of sequence-defined materials with reinforcement learning.* Princeton Materials Institute Symposium, Princeton, NJ. 2025, April.

Oliver, W., & Webb, M. A. *Controlled structure formation of sequence-defined materials with reinforcement learning.* APS Global Physics Summit, Anaheim, CA. 2025, March.

Oliver, W., & Webb, M. A. *When B_2 is not enough: Discriminating sequence determinants of attractive but non-phase separating intrinsically disordered proteins.* Rutgers-Princeton Biomolecular Condensates Day, Princeton, NJ. 2023, September.