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Princeton, NJ 08540

Wesley Oliver

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Education

Princeton University — Princeton, NJ
Ph.D., Chemical and Biological Engineering — expected May 2027
Advisor: Michael Webb, Ph.D.

Purdue University — West Lafayette, IN
B.S., Chemical Engineering — December 2021
GPA: 4.0/4.0

Research Experience

Graduate Research Assistant — Princeton, NJ
Princeton University — January 2023-Present

- *Advisor:* Professor Michael Webb
- My research focuses on combining molecular simulation and machine learning to accelerate property prediction and inverse design of sequence-defined materials, including proteins and polymers
- Create novel "physically-informed" features that improve the ability of machine learning models to predict protein properties
- Develop machine learning 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 (adaptive biasing force) and free energy calculations (thermodynamic integration, free energy perturbation)
- Developed expertise with tools such as LAMMPS and GROMACS to perform all-atom and coarse-grained molecular simulations
- Simulated all-atom systems of DNA to understand how incorporation of non-canonical base pairs influences DNA structure
- Collaborate with experimentalists to corroborate experimental findings using simulation data
- Use reinforcement learning control over molecular simulations to influence the morphology of sequence-defined materials
- Conduct high-throughput, active-learning campaign to explore the thermodynamic-dynamic tradeoff in intrinsically disordered protein design across coarse-grained models

Undergraduate Research Assistant — West Lafayette, IN
Purdue University — August 2019-December 2021

- *Advisor:* Professor David Corti
- Conducted computational research on the estimation of Hamaker constants, a value that quantifies the strength of van der Waals interactions
- Used a mathematical model of atomic force microscope (AFM) force experiments to investigate the impact of considering repulsive forces on these constants
- Research findings led to a peer-reviewed publication

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 (FEP, TI), all-atom and coarse-grained MD

Industry Experience

Process Research and Development Intern — Caldwell, ID
The J. R. Simplot Company — 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 — Williston, ND
ExxonMobil — 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 — Princeton, NJ
Prison Teaching Initiative — 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, NJ
Princeton University — Springs 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.