Alex M. Maldonado, PhD

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Ph.D. computational biochemist and software engineer with extensive experience developing and applying novel machine learning frameworks to problems in drug discovery and molecular simulation.

Education

Ph.D. in Chemical Engineering | *University of Pittsburgh* 2018 – 2023

- *Dissertation:* "Toward Robust and Efficient Atomistic Modeling of Solvent Effects"
- *Courses of Study:* Computational Structural Biology, Quantum Mechanics, Computational Chemistry, Nanoscale Modeling and Simulation, Statistical Mechanics, Biophysics

B.S.E. in Chemical Engineering | *Western Michigan University* 2013 – 2018

- *Thesis:* "Large-Scale Production of Immunobiosensors"
- *Minors:* Biomedical Sciences, Chemistry, and Mathematics
- *Courses of Study:* Physical Chemistry, Bioprocess Engineering, Linear Algebra, Differential Equations, Thermodynamics and Kinetics, Transport Phenomena, Human Physiology, Microbiology, Genetics

Experience

University of Pittsburgh

Assistant Teaching Professor Aug 2025 – Present

- Design and instruct four undergraduate courses, including biochemistry, computational biology, and authentic research experience in computational biology.
- Use molecular simulations, machine learning, and virtual screening to investigate protein dynamics and protein-ligand interactions.
- Engage over 200 students annually through a dynamic, project-based curriculum featuring hands-on computational labs and critical analysis of primary research literature.
- Mentored students through semester-long group research projects and the authorship of scientific perspective articles, developing their proficiency in advanced programming and data interpretation.

Postdoctoral Associate May 2023 – Aug 2025

- Developed reproducible frameworks for force field parameterization.
- Spearheaded collaborative projects spanning structural biology, drug design, and gene therapy.
- Created and maintained research software tools using Python, Mojo, TypeScript, and Rust.
- Taught undergraduate courses computational biology during Fall and Spring semesters.
- Mentored graduate and undergraduate students in computational biology research.

Graduate Student Researcher Aug 2018 – Apr 2023

- Architected a novel many-body Gradient-Domain Machine Learning (mbGDML) framework in Python, enabling the creation of quantum-accurate, size-transferable force fields from minimal training data.
- Pioneered a systematic investigation to quantify and benchmark uncertainties across a suite of advanced solvation models (e.g., QM/MM, PCM, COSMO-RS, ESM-RISM).
- Developed and containerized a suite of reusable Python tools for high-throughput computational chemistry, integrating libraries like NumPy, PyTorch, and PySCF to automate reaction discovery and alchemical free energy workflows.

Technical Expertise

Languages: Python, Mojo, Rust, TypeScript

Scientific Computing: Polars, NumPy, pandas, PyArrow, Apache Spark, Ray, Docker, Spack, SLURM

Molecular Modeling

- **Simulation:** Amber, OpenMM, ASE, QM/MM
- **Methods:** Alchemical simulations, replica exchange, metadynamics, umbrella sampling, nudged elastic band, gaussian accelerated molecular dynamics, growing string method
- **Quantum Chemistry:** ORCA, PySCF, xTB, Psi4

Machine Learning: PyTorch, scikit-learn, Deep Graph Library, UMAP

Visualization: Matplotlib, PyMOL, ChimeraX, VMD, Illustrator, p5.js

Selected Publications

Rosenbaum, J. C.; **Maldonado, A. M.**; Durrant, J. D.; Carlson, A. E. A genetically encoded probe pushes copper sensing into the sub-femtomolar range. *Under review*.

Kochnev, Y.; Ahmed, M.; **Maldonado, A. M.**; Durrant, J. D. MolModa: Accessible and secure molecular docking in a web browser. *Nucleic Acids Res.* **2024**, *52* (W1), W498–W506. DOI: 10.1093/nar/gkae406

Maldonado, A. M.; Vassilev-Galindo, V.; Poltavsky, I.; Tkatchenko, A.; Keith, J. A. Modeling molecular ensembles with gradient-domain machine learning force fields. *Digital Discovery*. **2023**, *2* (3), 871–880.DOI: 10.1039/D3DD00011G

Maldonado, A. M.; Hagiwara, S.; Choi, T. H.; et al. Quantifying uncertainties in solvation procedures for modeling aqueous phase reaction mechanisms. *J. Phys. Chem. A* **2021**, *125* (1), 154–164. DOI: 10.1021/acs.jpca.0c08961

Selected Software

simplify	*github.com/scienting/simlify*	A simulation framework to streamline the development and execution of computational models.
atomea	*github.com/scienting/atomea*	A uniform, hierarchical data model for atomistic systems built on Zarr and Parquet files.
raygent	*github.com/scienting/raygent*	Parallelize computations and data analysis with directed acyclic graphs powered by Ray.
povme	*github.com/durrantlab/povme*	Protein pocket shape analysis for ensemble docking.

Honors and Awards

Pitt Chancellor's Teaching Fellowship	2025
Pitt Provost's Dissertation Fellowship	2022 – 2023
R. K. Mellon Graduate Fellowship	2020 – 2022
Pitt STRIVE Scholar Fellowship	2018 – 2020
NSF GRFP Honorable mention	2018