Alex **Maldonado**

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Research

University of Pittsburgh *Pittsburgh, Pennsylvania*

Postdoctoral Associate (Biological Sciences) *May 2023 - Present*

- Train on-the-fly machine learning force fields for enhanced sampling with active learning.
- Develop an automatable and scalable classical force field parameterization scheme for biomolecules.
- Analyze protein-protein and protein-ligand interactions with molecular simulations and machine learning.

Graduate Student Researcher (Chemical Engineering) *Aug. 2018 - Apr. 2023*

- Designed, trained, and analyzed machine learning force fields on explicitly solvated systems.
- Employed implicit, explicit, and mixed implicit/explicit solvation modeling techniques.
- Modeled reaction mechanisms with quantum chemical methods and molecular simulations.
- Implemented knowledge documentation practices, created training materials, and standardized data management.

Western Michigan University *Kalamazoo, Michigan*

Undergraduate Student Researcher (Chemical Engineering) *Mar. 2016 - Jun. 2018*

- Designed, executed, and analyzed experiments to develop point-of-use biosensors.
- Quantified protein concentrations using UV-Vis spectroscopy and Bradford assay.
- Designed crosslinking procedure with EDC to improve adsorption of antibodies to biosensors.

Education

University of Pittsburgh *Pittsburgh, Pennsylvania*

Ph.D. in Chemical Engineering *Apr. 2023*

- Dissertation: Toward robust and efficient atomistic modeling of solvent effects.
- Advisor: John A. Keith

Western Michigan University *Kalamazoo, Michigan*

B.S.E. in Chemical Engineering *Apr. 2018*

Minors: Biological Sciences and Mathematics

- Design Project: Design and evaluation of a large-scale biosensor manufacturing process.
- Advisor: Brian R. Young

Teaching

University of Pittsburgh *Pittsburgh, Pennsylvania*

Instructor *Fall 2023 - Present*

- BIOSC 1540 - Computational biology (2024s; Undergraduate)
- BIOSC 1630 - Computational biology seminar (2023f; Undergraduate)

Teaching Assistant *Summer 2020 - Spring 2022*

- CHE 2101 - Fundamentals of thermodynamics (2022s, 2021s; Graduate)
- CHE 0400 - Reactive process engineering (2020sm; Undergraduate)

INVESTING NOW *Pittsburgh, Pennsylvania*

Instructor *May 2019 – Aug. 2019*

- Prepared syllabus and hands-on activities for a five-week course about energy and sustainability.
- Led classes, discussions, and activities for 11th-grade historically underrepresented students.

Service

Ingenium *Pittsburgh, Pennsylvania*
Reviewer *Aug. 2018 – Apr. 2021*

- Graduate student reviewer for undergraduate research journal in Pitt Swanson School of Engineering.

AIChE National Conference *Pittsburgh, Pennsylvania*
Poster Judge *Oct. 2018*

- Graduate student poster judge for AIChE topical conference.

Presentations

Pitt Chemical and Petroleum Engineering Research Day *Pittsburgh, Pennsylvania*
Towards atomistic modeling of complex environments with many-body machine learning potentials *Sep. 1, 2022*

American Chemical Society National Conference *Virtual*
Modeling solvents with many-body, gradient-domain machine learning force fields *Aug. 22, 2021*

American Institute of Chemical Engineering National Conference *Virtual*
Many-body machine learning force fields for explicit solvent modeling *Jul. 19, 2020*

Publications

† denotes equal contributions.

10. Rosenbaum, J. C.; **Maldonado, A. M.**; Durrant, J. D.; Carlson, A. E. Sensitive and ratiometric copper detection using a fluorescent protein. *In preparation*. metalflare.oasci.org
9. Ahmed, M.;† **Maldonado, A. M.**;† Durrant, J. D. From byte to bench to bedside: Molecular dynamics simulations and drug discovery. *BMC Biology*. **2023**, *21* (1), 299. DOI: 10.1186/s12915-023-01791-z
8. **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
7. Eikey, E. A.; **Maldonado, A. M.**; Griego, C. D.; Von Rudorff, G. F.; Keith, J. A. Quantum alchemy beyond singlets: Bonding in diatomic molecules with hydrogen. *J. Chem. Phys.* **2022**, *156* (20), 204111. DOI: 10.1063/5.0079487
6. Eikey, E. A.; **Maldonado, A. M.**; Griego, C. D.; Von Rudorff, G. F.; Keith, J. A. Evaluating quantum alchemy of atoms with thermodynamic cycles: Beyond ground electronic states. *J. Chem. Phys.* **2022**, *156* (6), 064106. DOI: 10.1063/5.0079483
5. Griego, C. D.;† **Maldonado, A. M.**;† Zhao, L.; et al. Computationally guided searches for efficient catalysts through chemical/materials space: Progress and outlook. *J. Phys. Chem. C* **2021**, *125* (16), 6495–6507. DOI: 10.1021/acs.jpcc.0c11345
4. **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
3. **Maldonado, A. M.**; Basdogan, Y.; Berryman, J. T.; Rempe, S. B.; Keith, J. A. First principles modeling of chemistry in mixed solvents: Where to go from here? *J. Chem. Phys.* **2020**, *152* (13), 130902. DOI: 10.1063/1.5143207
2. Basdogan, Y.; **Maldonado, A. M.**; Keith, J. A. Advances and challenges in modeling solvated reaction mechanisms for fuels and renewable chemicals. *WIREs Comput. Mol. Sci.* **2020**, *10* (2), e1446. DOI: 10.1002/wcms.1446
1. **Maldonado, A. M.**; Keith, J. A.; Schwarz, K.; Sundararaman, R. Solvation effects in first-principles calculations for catalysis. In *Computational catalysis*, 2nd ed.; Janik, M. J., Asthagiri, A., Eds.; Royal Society of Chemistry. *In press*.

Honors and awards

2022 **Best Oral Presentation**; Chemical and Petroleum Engineering Research Day, University of Pittsburgh
2022 – 2023 **Dissertation Year Fellowship**; Office of the Provost, University of Pittsburgh
2020 – 2022 **R. K. Mellon Graduate Fellowship**; University of Pittsburgh Center for Energy

2018	**Honorable mention**; Graduate Research Fellowships Program, National Science Foundation
2018 – 2020	**Scholar fellowship**; STRIVE program, University of Pittsburgh
2017 – 2018	**Summer Research Experience**; LSAMP, Western Michigan University

Skills

Programming	Python, JavaScript, TypeScript, Bash
Machine learning	Hyperparameter tuning, neural networks, clustering, dimensionality reduction, feature selection
Quantum chemistry	ORCA, xtb, Psi4, PySCF, MOLPRO, Gaussian
Molecular simulation	Amber, Atomic simulation environment, OpenMM
Rare-event sampling	Umbrella sampling, metadynamics, growing string method, nudged elastic band
Packages	PyTorch, NumPy, Ray, XGBoost, scikit-learn, pandas, pymoo, SciPy, UMAP
Graphic design	Inkscape, Scribus, p5.js, Adobe Photoshop, GIMP, Adobe Illustrator, Blender

Software development

SIMLIFY (Python) *gitlab.com/oasci/software/simlify*
Simplify and automate molecular simulation workflows.

ATOMEA (Python) *gitlab.com/oasci/software/atomea*
Extensible schema for atomistic simulations and calculations.

REPTAR (Python) *gitlab.com/oasci/software/reptar*
A tool for storing and analyzing manuscript-scale computational chemistry data.

MBGDML (Python) *github.com/keithgroup/mbGDML*
Package to automate creating, using, and analyzing many-body machine learning force fields.

CCLIB (Python) *github.com/cclib/cclib*
A library that provides parsers for output files of computational chemistry packages.

OBSIDIAN BIBTEX ADDER (TypeScript) *github.com/oasci/obsidian-bibtex-adder*
Obsidian plugin to add BibTeX entries from DOIs using the Crossref REST API.