Alex Maldonado

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Education

2018 – Present **PhD in Chemical Engineering** — University of Pittsburgh
Adviser: John A. Keith; GPA: 3.8/4.0.

4/2018 **BS in Chemical Engineering** — Western Michigan University
Senior Design Project: Design and evaluation of a large-scale biosensor manufacturing process.
Adviser: Brian R. Young; GPA: 3.6/4.0.

Research Experience

2018 – Present **Graduate Researcher** — University of Pittsburgh

- Developed transferable many-body gradient domain machine learning force fields with collaborators at the University of Luxembourg.
- Employed computational quantum chemistry to predict solvated reaction mechanisms with implicit, mixed implicit/explicit, and explicit solvent methods.
- Implemented knowledge documentation practices, prepared training materials, and standardized data management procedures.

2016 – 2018 **Undergraduate Researcher** — Western Michigan University
Developed protocol for small-scale manufacturing of novel point-of-use immunodiagnostic device.

Software Development

2020 – Present **Many-Body Gradient Domain Machine Learning (mbgdml)** — github.com/keithgroup/mbGDML
Python package to create, use, and analyze many-body gradient domain machine learning force fields.

2019 – Present **Computational Chemisty Library (cclib)** — github.com/cclib/cclib
A Python library that provides parsers for output files of computational chemistry packages.

Teaching

2020 **Teaching Assistant** — University of Pittsburgh
Thermodynamics (CHE 2101; Spring 2021)

- Graded assignments and hosted office hours.

Reaction Engineering (CHE 400; Summer 2020)

- Updated and converted MATLAB assignments to Jupyter notebooks.
- Designed, prepared, and executed a new module on bioreaction engineering.

2019 **Instructor — INVESTING NOW** — University of Pittsburgh

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

Service

2018 – Present **Reviewer — Ingenium** — Pittsburgh, PA
Graduate student reviewer for undergraduate research journal in Pitt Swanson School of Engineering.

2018 **Poster Judge — AIChE National Conference** — Pittsburgh, PA
Graduate student poster judge for AIChE topical conference.

2016 – 2018 **Member — Environmental Concerns Committee** — Kalamazoo, MI
Advised city manager and city commission regarding environmental matters and served as a citizens' forum.

Awards

2021	R. K. Mellon Graduate Fellowship	University of Pittsburgh Center for Energy
2020	Honorable Mention - Graduate Research Fellowship Program	National Science Foundation
2018	Pitt STRIVE Scholar	University of Pittsburgh
2017	MI-LSAMP	Western Michigan University

Presentations

7/19/2020 — 2020 AIChE National Conference (Oral) — Virtual
Many-body machine learning force fields for explicit solvent modeling (prerecorded video).

3/24/2018 — 2018 ASEE NCS Conference (Oral) — The University of Akron; Akron, OH
Utilization of Bradford assay to aid in development of a novel point-of-use immunobiosensor.

Publications

4. Griego, C.*, **Maldonado, A. M.***, Zhao, L., et al. Computationally guided searches for efficient catalysts through chemical/materials space: progress and outlook. *J. Phys. Chem. C. In press*.
3. **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*. DOI: 10.1021/acs.jpca.0c08961
2. **Maldonado, A. M.**, Basdogan, Y., Berryman, J. T., Rempe, S. B., Keith, J. A. (2020) First principles modeling of chemistry in mixed solvents: Where to go from here? *J. Chem. Phys.*, *152*(13), 130902. DOI: 10.1063/1.5143207
1. Basdogan, Y., **Maldonado, A. M.**, Keith, J. A. (2020) Advances and challenges in modeling solvated reaction mechanisms for fuels and renewable chemicals. *WIREs Comput. Mol. Sci.*, *10*(2), e1446. DOI: 10.1002/wcms.1446.

Technical Skills

Languages: Python, Bash.

Packages: NumPy, SciPy, cclib.

Tools: Git, GitHub, Jupyter.

Modeling: ORCA, Gaussian, xtb, NAMD, molecularGSM, ABCluster.

Visualization: Blender, Inkscape, Illustrator, VMD, matplotlib.