

# Alex Maldonado

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## Education

2018 – Present	PhD in Chemical Engineering Adviser: John A. Keith; GPA: 3.8/4.0.	University of Pittsburgh
4/2018	BS in Chemical Engineering Senior Design Project: Design and evaluation of a large-scale biosensor manufacturing process. Adviser: Brian R. Young; GPA: 3.6/4.0.	Western Michigan University

## Research Experience

2018 – Present	Graduate Researcher <ul style="list-style-type: none"><li>Developed transferable many-body gradient domain machine learning force fields with collaborators at the University of Luxembourg.</li><li>Employed computational quantum chemistry to predict solvated reaction mechanisms with implicit, mixed implicit/explicit, and explicit solvent methods.</li><li>Implemented knowledge documentation practices, prepared training materials, and standardized data management procedures.</li></ul>	University of Pittsburgh
2016 – 2018	Undergraduate Researcher Developed protocol for small-scale manufacturing of novel point-of-use immunodiagnostic device.	Western Michigan University

## Software Development

2021	Quantum chemistry JSON (qcjson) Convert computational chemistry output files to standardized JSON files.	<a href="https://github.com/keithgroup/qcjson">github.com/keithgroup/qcjson</a>
2020	Many-Body Gradient Domain Machine Learning (mbgdml) Python package to create, use, and analyze many-body gradient domain machine learning force fields.	<a href="https://github.com/keithgroup/mbGDML">github.com/keithgroup/mbGDML</a>
2019	Computational Chemistry Library (cclib) A Python library that provides parsers for output files of computational chemistry packages.	<a href="https://github.com/cclib/cclib">github.com/cclib/cclib</a>

## Teaching

2020	Teaching Assistant Thermodynamics (CHE 2101; Spring 2021) <ul style="list-style-type: none"><li>Graded assignments and hosted office hours.</li></ul> Reaction Engineering (CHE 400; Summer 2020) <ul style="list-style-type: none"><li>Updated and converted MATLAB assignments to Jupyter notebooks.</li><li>Designed, prepared, and executed a new module on bioreaction engineering.</li></ul>	University of Pittsburgh
2019	Instructor – INVESTING NOW <ul style="list-style-type: none"><li>Prepared syllabus and hands-on activities for a five-week course about engineering and sustainability.</li><li>Led classes, discussions, and activities for 11th grade historically underrepresented students.</li></ul>	University of Pittsburgh

## Service

2018 – Present	Reviewer – Ingenium Graduate student reviewer for undergraduate research journal in Pitt Swanson School of Engineering.	Pittsburgh, PA
2018	Poster Judge – AIChE National Conference Graduate student poster judge for AIChE topical conference.	Pittsburgh, PA
2016 – 2018	Member – Environmental Concerns Committee Advised city manager and city commission regarding environmental matters and served as a citizens' forum.	Kalamazoo, MI

## 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) Many-body machine learning force fields for explicit solvent modeling (prerecorded video).	Virtual
3/24/2018	2018 ASEE NCS Conference (Oral) Utilization of Bradford assay to aid in development of a novel point-of-use immunobiosensor.	The University of Akron; Akron, OH

## Publications

4. Griego, C.\*, **Maldonado, A. M.\***, Zhao, L., et al. (2021). Computationally guided searches for efficient catalysts through chemical/materials space: Progress and outlook. *J. Phys. Chem. C*.  
<https://doi.org/10.1021/acs.jpcc.0c11345>.
3. **Maldonado, A. M.**, Hagiwara, S., Choi, T. H., et al. (2021). Quantifying uncertainties in solvation procedures for modeling aqueous phase reaction mechanisms. *J. Phys. Chem. A*, 125(1), 154-164.  
<https://doi.org/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.  
<https://doi.org/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.  
<https://doi.org/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.