Michael G. Taylor, Ph.D.

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Researcher interested in bringing molecular/materials modeling and data-driven discovery to real and emerging materials.

Education

Aug. 2019 **University of Pittsburgh**, Pittsburgh, PA.
Ph.D. in Chemical Engineering, Thesis: "Ligand-Protected Nanocluster Stability, Doping, and Prediction"

May 2013 **University of Nebraska-Lincoln**, Lincoln, NE.
B.S. in Chemical Engineering, *Cum Laude*

Work & Research

2019-Present **Massachusetts Institute of Technology (MIT), Department Chemical Engineering**, *Cambridge*, MA.
Postdoctoral Scholar, Advisor: Prof. Heather Kulik

- Leveraged *ab-initio* electronic structure methods toward rationalizing doping in In-P nanomaterials and towards tuning their stability and optical properties.
- Designed data mining workflow and MongoDB database of mononuclear transition metal complexes from the Cambridge Structural Database.
- Contributed ligand symmetry analysis, unique ID generation, and featurization routines generalized to all known experimental mononuclear octahedral transition metal complexes in the open-source molSimplify Python package for machine learning (ML)-accelerated analysis.
- Deliverables: 1 first-author peer-reviewed publication (1 in preparation), 1 conference presentation

2014-2019 **University of Pittsburgh, Department of Chemical and Petroleum Engineering**, *Pittsburgh*, PA.
Doctoral Researcher and National Science Foundation (NSF) Graduate Research Fellow (2016-2019), Advisor: Prof. Giannis Mpourmpakis

- Applied Density Functional Theory (DFT) methods to deepen understanding of the stability of metal nanoclusters and lead efforts on a reduced-cost model for screening the energetics of nanoalloys based on size, shape, composition, and chemical ordering.
- Calculated adsorption and facet-preference for growth modifiers of kidney stones, rationalizing dissolution mechanisms.
- Mentored 4 Undergraduates (1 co-author on publication) and 1 Masters Student (1st author publication)
- Deliverables: 6 first-author peer-reviewed publications, 9 co-author publications, 9 conference presentations

2013-2014 **Cargill Corn Milling North America**, *Blair*, NE.
Ethanol/Utilities Process Engineering Co-op

- Lead over $\$100,000$ in plant improvement projects.
- Created opportunities for data-driven plant operation using principal component (PCA) analyses of real-time data.

Summer 2012 **University of Pittsburgh**, *Pittsburgh*, PA.
NSF Research Experience for Undergraduates (REU) Fellow, Advisor: Prof. J. Karl Johnson

- Simulated desalination through carbon nanotube materials using Molecular Dynamics (MD)
- Deliverables: 1 peer-reviewed co-author publication and 1 conference presentation

Leadership

Fall 2020 **Grader, 10.637 - Quantum Chemical Simulation**, *MIT*, 13 Students.

- Lead live virtual laboratory exercises related to computational chemistry and quantum chemical simulations.

2015-2017 **Chemical Engineering Graduate Student Association (GSA) President**, *University of Pittsburgh.*

- **Organization:** Led and coordinated department-wide research day. Started joint happy hours initiative with Carnegie Mellon University department of chemical engineering 2015-2016. Coordinated recruiting events for incoming PhD students 2015-2017.
- **Volunteering:** Coordinated department educational outreach at the Engineer the Future and National Chemistry Day events at the Carnegie Science center in Pittsburgh with *at least 4,000 students*, 2016-2017.

2015-2017 **Teaching Assistant (x3), CHE 200 - Chemical Engineering Thermodynamics**, *University of Pittsburgh*, 70 Students.

- Lead five, 2-hour recitations and presented 2-hour lecture on excess properties.

Outreach & Professional Activities

2019-Present **Reviewer**.

- *Molecular Systems Design and Engineering*, *Inorganic Chemistry*

2017-2019 **Ingenium Graduate Student Editorial Board (x3)**, *Swanson School of Engineering*, University of Pittsburgh.

- Served on the editorial board of Ingenium, the School of Engineering undergraduate research publication.

May 2018 **Intel International Science and Engineering Fair (ISEF)**, *Pittsburgh, PA*.

- Served as a Grand Awards judge for the chemistry division with an emphasis on advances in computational chemistry.

Apr. 2017 **High school outreach presentation**, *Central Catholic High School*, Pittsburgh, PA.

- Presented my experience as a Chemical Engineer and scientist to a high school, pre-engineering class (around 50 students).

Skills & Interests

Computer

Languages	Proficiency: Python, BASH - Familiar: Fortran, Matlab, R
ML	Tensorflow/Keras, scikit-learn
Modeling	CP_2K (Molecular and Periodic DFT), Turbomole, TeraChem
Platforms	GNU/Linux (Redhat/Ubuntu), MacOS, Windows
Typesetting	LaTeX, Word (Microsoft Office)
Web	Github Pages/Jekyll - Familiar: Flask/JavaScript/CSS
Visualization	Blender, Inkscape/Illustrator, Bokeh, Pymol
Development	git, vim, VisualStudio
Personal	Hiking, Music (Trumpet), Brewing Mead

Awards & Grants

Oct. 2019 **Best Poster Award**, *Inorganometallic Catalyst Design Center (ICDC) annual meeting*, shared with Aditya Nandy).

Apr. 2019 **ChE Outstanding Research Assistant Award**, *Engineering Graduate Student Organization, University of Pittsburgh*.

Dec. 2018 **Dr. James M. Coull Memorial Fellowship Award**, *Department of Chemical and Petroleum Engineering University of Pittsburgh*, $1,500.

Oct. 2018 **CoMSEF Division Graduate Student Award**, *AIChE*, $250.

Dec. 2017 **Lead Extreme Science and Engineering Discovery Environment (XSEDE) Proposal**, *NSF*, $32,355.54.

Mar. 2017 **Best Poster Presentation (Travel Grant)**, *Advancing Research through Computing (ARC) Conference*, University of Pittsburgh, $500.

Apr. 2016 **Graduate Research Fellowship Program (GRFP)**, *NSF*, $120,000 Value.

Selected Publications

1. **M. G. Taylor, T. Yang, S. Lin, A. Nandy, J. P. Janet, C. Duan, and H. J. Kulik**, *"Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions"*, J. Phys. Chem. A, (2020).
2. **M. G. Taylor and G. Mpourmpakis.**, *"Thermodynamic Stability of Ligand-Protected Metal Nanoclusters"*, Nat. Comm., (2017).
2. **M. G. Taylor, N. Austin, C. E. Gounaris, and G. Mpourmpakis.**, *"Catalyst design based on morphology- and environment-dependent adsorption on metal nanoparticles"*, ACS Catal., (2015).