

Education

- May 2019 **Expected: Ph.D. Chemical Engineering**, *University of Pittsburgh*, Pittsburgh, PA.
Applied electronic structure methods to elucidate nanomaterials growth and stability.
Advisor: Giannis Mpourmpakis
- May 2013 **B.S. Chemical Engineering**, *University of Nebraska-Lincoln*, Lincoln, NE.
Cum Laude

Research Experience

- 2014-Present **PhD. Graduate Research Assistant**, *University of Pittsburgh, Department of Chemical and Petroleum Engineering*, Pittsburgh, PA.
Atomically-precise nanoparticle growth and stability
I apply Density Functional Theory (DFT) methods and chemical structure analysis techniques to understand the stability and growth of metal nanoclusters. Beyond monometallic clusters I have looked into doping and growth of bimetallic clusters and the resultant shift in electronic properties. I am using our findings to focus on computational design of metal nanoclusters.
Rationalization of kidney stone growth modifier efficacy
I use DFT to calculate adsorption and facet-preference for different growth modifiers to kidney stones. I helped rationalize dissolution of kidney stones observed in experiments.
Stability of nanoalloys
I have helped develop a model for screening the stability of nanoalloys based on size, shape, composition, and chemical ordering descriptors. I apply this new model for nanoalloy design.
- Summer 2012 **NSF Research Experience for Undergraduates (REU) Fellow**, *University of Pittsburgh*, Pittsburgh, PA.
Advisor: J. Karl Johnson
Zwitterion-functionalized carbon nanotubes for desalination
I used Molecular Dynamics (MD) to explore efficient desalination in carbon nanotube materials.
- 2011–2013 **Undergraduate Research Assistant**, *University of Nebraska-Lincoln*, Lincoln, NE.
Functionalized chitosan microspheres for targeted DNA detection
- Summer 2010 **Undergraduate Research Assistant**, *Creighton University*, Omaha, NE.
Understanding inner-ear developmental biology in mouse models

Publications

- 2018 Z. Yan*, M. G. **Taylor***, A. Mascareno, and G. Mpourmpakis. “Size-, Shape-, and Composition-Dependent Model for Metal Nanoparticle Stability Prediction”. In: *Nano Letters* 18.4 (2018), pp. 2696–2704. DOI: 10.1021/acs.nanolett.8b00670.
- 2017 Q. Li, K. J. Lambright, M. G. **Taylor**, K. Kirschbaum, T.-Y. Luo, J. Zhao, G. Mpourmpakis, S. Mokashi-Punekar, N. L. Rosi, and R. Jin. “Reconstructing the Surface of Gold Nanoclusters by Cadmium Doping”. In: *Journal of the American Chemical Society* 139.49 (2017), pp. 17779–17782. DOI: 10.1021/jacs.7b11491.
- Q. Li, M. G. **Taylor**, K. Kirschbaum, K. J. Lambright, X. Zhu, G. Mpourmpakis, and R. Jin. “Site-selective substitution of gold atoms in the Au₂₄(SR)₂₀ nanocluster by silver”. In: *Journal of Colloid and Interface Science* 505 (1 Nov 2017 2017), pp. 1202–1207. DOI: 10.1016/j.jcis.2017.06.049.
- M. G. **Taylor** and G. Mpourmpakis. “Thermodynamic Stability of Ligand-Protected Metal Nanoclusters”. In: *Nature Communications* 8 (May 2017), p. 15988. DOI: 10.1038/ncomms15988.

Q. Li*, T.-y. Luo*, M. G. **Taylor***, S. Wang, X. Zhu, Y. Song, G. Mpourmpakis, N. L. Rosi, and R. Jin. "Molecular "surgery" on a 23-gold-atom nanoparticle". In: *Science Advances* 3.5 (2017), e1603193. DOI: 10.1126/sciadv.1603193.

- 2016 J. Chung, I. Granja*, M. G. **Taylor***, G. Mpourmpakis, J. R. Asplin, and J. D. Rimer. "Molecular modifiers reveal a mechanism of pathological crystal growth inhibition". In: *Nature* 536.7617 (2016), pp. 446–450. DOI: 10.1038/nature19062.
- 2015 M. G. **Taylor***, N. Austin*, C. Gounaris, and G. Mpourmpakis. "Catalyst Design Based on Morphology and Environment Dependent Adsorption on Metal Nanoparticles". In: *ACS Catalysis* 5.11 (2015), pp. 6296–6301. DOI: 10.1021/acscatal.5b01696.
- 2013 W. Chan, H.-y. Chen, A. Surapathi, M. G. **Taylor**, X. Shao, E. Marand, and J. K. Johnson. "Zwitterion Functionalized Carbon Nanotube / Polyamide Nanocomposite Membranes for Water Desalination". In: *ACS Nano* 7.6 (2013), pp. 5308–5319. DOI: 10.1021/nn4011494.

* Indicates authors contributed equally to this work

Awards and Grants

- Dec. 2017 **Lead: Extreme Science and Engineering Discovery Environment (XSEDE) Proposal, National Science Foundation (NSF)**, \$32,355.54.
- Mar. 2017 **Best Poster Presentation, Advancing Research through Computing (ARC) Conference**, University of Pittsburgh, \$500 Travel Grant.
- Jan. 2017 **University of Pittsburgh GPSG Travel Grant, \$500.**
- Dec. 2016 **Contributed: XSEDE Proposal, NSF**, \$28,015.28.
- Apr. 2016 **Graduate Research Fellowship Program (GRFP) - Awarded**, NSF, \$34,000 Stipend + \$12,000 Tuition Waiver for 3 Years.
- Dec. 2015 **Contributed: XSEDE Proposal, NSF**, \$83,860.70.
- Apr. 2015 **GRFP - Honorable Mention, NSF.**

Presentations

- 2018 M. G. Taylor, Z. Yan, A. Mascareno, and G. Mpourmpakis, *Bond-Centric Model for Metal Nanoparticle Energetics*, **Poster presentation**, Pittsburgh Cleveland Catalysis Society (PCCS), Pittsburgh, PA, USA. 8 June 2018.
- M. G. Taylor and G. Mpourmpakis, *Rationalizing Stability of Atomically-precise, Ligand-protect Nanoclusters*, **Oral presentation**, Department of Chemical and Petroleum Engineering Research Day 2018, Pittsburgh, PA, USA. 20 February 2018.
- 2017 M. G. Taylor and G. Mpourmpakis, *Stability and Prediction of Thiolated Metal Nanoclusters*, **Poster presentation**, Advancing Research through Computing (ARC) Conference, Pittsburgh, PA, USA. 2 March 2017.
- 2016 M. G. Taylor and G. Mpourmpakis, *Structure-Dependent Stability of Magic-Number Thiolated Metal Nanoparticles*, **Oral presentation**, AIChE Annual Meeting 2016, San Francisco, CA, USA. 16 November 2016.
- M.G. Taylor, J. Chung, J. D. Rimer, and G. Mpourmpakis, *Elucidating the Mechanisms for Kidney Stone GRowth Inhibition and Dissolution*, **Poster presentation**, Department of Chemical and Petroleum Engineering Research Day 2016, Pittsburgh, PA, USA. 25 October 2016.
- M. G. Taylor and G. Mpourmpakis, *Modeling the structure-dependent stability of thiolated metal nanoparticles*, **Oral presentation**, ACS Fall National Meeting 2016, Philadelphia, PA, USA. 23 August 2016.
- M. G. Taylor and G. Mpourmpakis, *Exploring the Structure-Dependent Stability of Thiolated Metal Nanoparticles*, **Poster presentation**, Midwest Theoretical Chemistry Conference (MWTCC) 2016, Pittsburgh, PA, USA. 9 June 2016.

- 2015 M.G. Taylor, J. Chung, I. Carnaval, J. D. Rimer and G. Mpourmpakis, *Kidney Stone Growth Modification: Insights from First Principles Calculations*, **Oral presentation**, AIChE Annual Meeting 2015, Salt Lake City, UT, USA. 12 November 2015.
- M. G. Taylor, J. Chung, I. Carnaval, J. D. Rimer, and G. Mpourmpakis, *Kidney Stone Growth Modification: Insights from First Principles*, **Oral presentation**, Carnegie Mellon University - Pittsburgh Simulator's Meeting 2015, Pittsburgh, PA, USA. 20 May 2015.
- M. G. Taylor, J. Chung, I. Carnaval, J. D. Rimer, and G. Mpourmpakis, *Kidney Stone Growth Modification: Insights from First Principles*, **Poster presentation**, Department of Chemical and Petroleum Engineering Research Day 2015, Pittsburgh, PA, USA. 17 March 2015.
- 2012 M. G. Taylor, H-y. Chen, and J. K. Johnson, *Zwitterion-Functionalized CNTs for Efficient Desalination*, **Poster presentation**, AIChE Annual Meeting 2012 - Student Session, Pittsburgh, PA, USA. 29 October 2012.

Leadership, Outreach, and Broader Impacts

- May 2018 **Intel International Science and Engineering Fair (ISEF)**, Pittsburgh, PA.
Served as a grad awards judge for the chemistry division with an emphasis on advances in computational chemistry.
- 2015-2017 **Chemical Engineering Graduate Student Association (GSA) President**, University of Pittsburgh.
Organization: Led the department research day 2016. Started and coordinated joint happy hours with Carnegie Mellon University department of chemical engineering 2015-2016. Helped coordinate recruiting events for incoming PhD students 2015-2017.
Volunteering: Co-coordinated department involvement in 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. Helped lead volunteer efforts to clean the city of Pittsburgh.
- 2017-2018 **Ingenium editorial board**, Swanson School of Engineering, University of Pittsburgh.
Served on the editorial board as a reviewer for Ingenium, the school of engineering undergraduate publication.
- Apr. 2017 **High school outreach presentation**, Central Catholic High School, Pittsburgh, PA.
Presented an informative and motivational talk on my experiences as a chemical engineer and as a scientists to a high school, pre-engineering class of around 50 students.
- Apr. 2016 **Undergraduate research seminar presentation**, University of Pittsburgh, Department of Chemical Engineering.
Presented my research and experiences in graduate school to the undergraduates in the department towards inspiring and influencing them towards careers in science.
- Apr. 2015 **ISEF**, Pittsburgh, PA.
Served as volunteer for safety and initial inspection of posters at the international high-school science fair.

Teaching and Advising Experience

- 2015-2018 **Research mentoring and advising**.
Undergraduates: Isadora Carnaval (2015), Peter Tancini (2015-2016), John Hoover (2016), Ashley Mascareno (Summer 2017) (Co-Author on publication)
Masters: Zihao Yan (2016-2018) (1st author publication)
- Spring 2017 **Teaching Assistant, CHE 200 - Chemical Engineering Thermodynamics**, University of Pittsburgh, 70 Students.
Lead five, 2-hour recitations on problem solving and further conceptual understanding.
Presented 2-hour lecture on excess properties and the thermodynamics of mixtures, connected these properties to cutting-edge research.
- Spring 2016 **Teaching Assistant, CHE 200 - Chemical Engineering Thermodynamics**, University of Pittsburgh, 70 Students.

Presented 2-hour lecture on chemical equilibrium and chemical potential.

Spring 2015 **Teaching Assistant, CHE 200 - Chemical Engineering Thermodynamics**, *University of Pittsburgh*, 70 Students.

Computing

Languages	Python, FORTRAN, UNIX shell (BASH), ASE package, R, MATLAB
Modeling	CP ₂ K, Turbomole, LAMMPS, DFTB+
Platforms	GNU/Linux, MacOS, Windows
Web	Github Pages/Jekyll
Visualization	Blender, GIMP, Origin, Inkscape
Development	git, vim

Relevant Graduate Coursework

Spring 2017	CMCHE 0611 , <i>Computer Science for Chemical Engineers</i> .
Fall 2016	IE 3097 , <i>Algorithms for Engineers</i> .
Fall 2016	CHEM 2620 , <i>Atoms, Molecules, and Materials</i> .
Spring 2016	CHE 3460 , <i>Advanced Scientific Visual Communication</i> .
Fall 2015	STAT 2270 , <i>Data Mining</i> .
Fall 2015	MSE 2003 , <i>Structure of Materials</i> .
Spring 2015	CHE 2017 , <i>Chemical Energy and the Nature of the Chemical Bond</i> .