

Education

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

Research Experience

- 2014-Present **PhD. Candidate**, *University of Pittsburgh, Department of Chemical and Petroleum Engineering*, Pittsburgh, PA.
Atomically-precise nanoparticle growth and stabilization
Apply Density Functional Theory (DFT) methods to understand the stability and growth of metal nanoclusters. Findings used to develop methods for rapid computational design of hypothetical metal nanoclusters.
Stability and chemical reactivity of nanoalloys
Created a new model for screening the energetics of nanoalloys based on size, shape, composition, and chemical ordering. Currently applying this new model for metal nanoparticle and nanoalloy design.
Kidney stone growth modifier efficacy
Calculated adsorption and facet-preference for different growth modifiers to kidney stones helping rationalize dissolution of kidney stones observed in experiments.
- Summer 2012 **NSF Research Experience for Undergraduates (REU) Fellow**, *University of Pittsburgh*, Pittsburgh, PA.
Advisor: J. Karl Johnson
Zwitterion-functionalized carbon nanotubes for desalination
Applied Molecular Dynamics (MD) to understanding desalination through 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

- [1] N. Isenberg, M. G. Taylor, C. L. Hanselman, Z. Yan, G. Mpourmpakis, and C. Gounaris. “Accurate low-cost nanoparticle energetics and global optimization via tuned bond-cutting model.” In: *Targeted to Nature Communications* (2018), *Under Preparation*.
- [2] W. Li, M. G. Taylor, S. Mozaffari, S. Ivanov, S. Seifert, B. Lee, N. Shanaiah, Y. Lu, L. Kovarik, G. Mpourmpakis, and A. M. Karim. “Solvent Manipulation of the Pre-reduction Metal-Ligand Complex for Controlled Growth of Pd Nanoparticle.” In: *Targeted to Journal of the American Chemical Society* (2018), *Under Preparation*.
- [3] M. G. Taylor and G. Mpourmpakis. “Rethinking Heterometal Doping in Ligand-Protected Metal Nanoclusters.” In: *Journal of Physical Chemistry Letters* (2018), *Just Accepted*. DOI: 10.1021/acs.jpcllett.8b02679.
- [4] J. Chung, M. G. Taylor, I. Granja, J. R. Asplin, G. Mpourmpakis, and J. D. Rimer. “Factors Differentiating the Effectiveness of Polyprotic Acids as Inhibitors of Calcium Oxalate Crystallization in Kidney Stone Disease”. In: *Crystal Growth & Design* (2018), acs.cgd.8b00945. ISSN: 1528-7483. DOI: 10.1021/acs.cgd.8b00945. URL: <http://pubs.acs.org/doi/10.1021/acs.cgd.8b00945>.

- [5] M. G. Taylor*, Z. Yan*, 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.
- [6] Q. Li, K. J. Lambricht, 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.
- [7] Q. Li, M. G. Taylor, K. Kirschbaum, K. J. Lambricht, 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 (2017), pp. 1202–1207. DOI: 10.1016/j.jcis.2017.06.049.
- [8] M. G. Taylor and G. Mpourmpakis. “Thermodynamic Stability of Ligand-Protected Metal Nanoclusters”. In: *Nature Communications* 8 (2017), p. 15988. DOI: 10.1038/ncomms15988.
- [9] M. G. Taylor*, Q. Li*, T.-y. Luo*, 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.
- [10] J. Chung, M. G. Taylor*, I. Granja*, 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.
- [11] 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.
- [12] 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

- Apr. 2016 **Graduate Research Fellowship Program (GRFP) - Awarded** , NSF, \$34,000 Stipend + \$12,000 Tuition Waiver for 3 Years.
- Oct. 2018 **CoMSEF Division Graduate Student Award (in recognition of substantial contributions to computational molecular sciences)** , AIChE , \$500.
- Dec. 2017 **Led: Extreme Science and Engineering Discovery Environment (XSEDE) Proposal**, *National Science Foundation (NSF)*, \$32,355.54.
- Apr. 2015 **GRFP - Honorable Mention**, NSF.
- Mar. 2017 **Best Poster Presentation (Travel Grant)**, *Advancing Research through Computing (ARC) Conference*, University of Pittsburgh, \$500.
- Jan. 2017 **GPSG Travel Grant**, *University of Pittsburgh*, \$500.
- Dec. 2016 **XSEDE Proposal (Contributed)**, NSF, \$28,015.28.
- Dec. 2015 **XSEDE Proposal (Contributed)**, NSF, \$83,860.70.
- Summer 2012 **Research Experience for Undergraduates (REU) Fellow**, NSF.

Oral Presentations

- [1] M. G. Taylor, Z. Yan, A. Mascareno, and G. Mpourmpakis. Development of a Bond-Centric Model Thermodynamic Stability of Nanoalloys. AICHE Annual Meeting 2018, Pittsburgh, PA, USA. 28 October 2018.
- [2] M. G. Taylor, Q. Li, R. Jin, and G. Mpourmpakis. Rationalizing Stability and Doping of Atomically Precise Ligand-Protected Metal Nanoclusters. AICHE Annual Meeting 2018, Pittsburgh, PA, USA. 30 October 2018.

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- [3] M. G. Taylor, Z. Yan, A. Mascareno, and G. Mpourmpakis. Simple bond-centric model for accelerated nanoalloy energetics. ACS Fall National Meeting 2018, Boston, MA, USA. 19 August 2018.
- [4] M. G. Taylor, Q. Li, R. Jin, and G. Mpourmpakis. Molecular "surgery" and beyond: Understanding heterometal doping in atomically precise nanoclusters. ACS Fall National Meeting 2018, Boston, MA, USA. 21 August 2018.
- [5] M. G. Taylor and G. Mpourmpakis Rationalizing Stability of Atomically-precise, Ligand-protect Nanoclusters. Department of Chemical and Petroleum Engineering Research Day 2018, Pittsburgh, PA, USA. 20 February 2018
- [6] M. G. Taylor and G. Mpourmpakis. Structure-Dependent Stability of Magic-Number Thiolated Metal Nanoparticles. AIChE Annual Meeting 2016, San Francisco, CA, USA. 16 November 2016.
- [7] M. G. Taylor and G. Mpourmpakis. Modeling the structure-dependent stability of thiolated metal nanoparticles. ACS Fall National Meeting 2016, Philadelphia, PA, USA. 23 August 2016.
- [8] M. G. Taylor, J. Chung, I. Carnaval, J. D. Rimer and G. Mpourmpakis. Kidney Stone Growth Modification: Insights from First Principles Calculations. AIChE Annual Meeting 2015, Salt Lake City, UT, USA. 12 November 2015.
- [9] M. G. Taylor, J. Chung, I. Carnaval, J. D. Rimer, and G. Mpourmpakis Kidney Stone Growth Modification: Insights from First Principles. Carnegie Mellon University - Pittsburgh Simulator's Meeting 2015, Pittsburgh, PA, USA. 20 May 2015

Poster Presentations

- [1] M. G. Taylor and G. Mpourmpakis. Computer-Aided Description of Materials Stability at the Nanoscale. AIChE Annual Meeting 2018, Pittsburgh, PA, USA. 29 October 2018.
- [2] M. G. Taylor, Z. Yan, A. Mascareno, and G. Mpourmpakis Bond-Centric Model for Metal Nanoparticle Energetics. Pittsburgh Cleveland Catalysis Society (PCCS), Pittsburgh, PA, USA. 8 June 2018
- [3] M. G. Taylor and G. Mpourmpakis Stability and Prediction of Thiolated Metal Nanoclusters. Advancing Research through Computing (ARC) Conference, Pittsburgh, PA, USA. 2 March 2017
- [4] M. G. Taylor, J. Chung, J. D. Rimer, and G. Mpourmpakis Elucidating the Mechanisms for Kidney Stone Growth Inhibition and Dissolution. Department of Chemical and Petroleum Engineering Research Day 2016, Pittsburgh, PA, USA. 25 October 2016
- [5] M. G. Taylor and G. Mpourmpakis Exploring the Structure-Dependent Stability of Thiolated Metal Nanoparticles. Midwest Theoretical Chemistry Conference (MWTCC) 2016, Pittsburgh, PA, USA. 9 June 2016
- [6] M. G. Taylor, H-y. Chen, and J. K. Johnson Zwitterion-Functionalized CNTs for Efficient Desalination. AIChE Annual Meeting 2012 - Student Session, Pittsburgh, PA, USA. 29 October 2012
- [7] M. G. Taylor, J. Chung, I. Carnaval, J. D. Rimer, and G. Mpourmpakis Kidney Stone Growth Modification: Insights from First Principles. Department of Chemical and Petroleum Engineering Research Day 2015, Pittsburgh, PA, USA. 17 March 2015

Leadership, Outreach, and Broader Impacts

- 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.
- 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.

2017-2019 **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.

Professional Society Memberships

2012-Present **American Institute of Chemical Engineers (AIChE)**.

2015-Present **American Chemical Society (ACS)**.

2013-Present **Tau Beta Pi Engineering Fraternity**.

Computational Expertise

Languages Proficient in: Python, BASH, ASE package, R, MATLAB, Some experience in FORTRAN

Modeling CP₂K (Molecular and Periodic DFT), 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**, *Computer Science for Chemical Engineers*.
Fall 2016 **IE 3097**, *Algorithms for Engineers*.
Fall 2016 **CHEM 2620**, *Atoms, Molecules, and Materials*.
Spring 2016 **CHE 3460**, *Advanced Scientific Visual Communication*.
Fall 2015 **STAT 2270**, *Data Mining*.
Fall 2015 **MSE 2003**, *Structure of Materials*.
Spring 2015 **CHE 2017**, *Chemical Energy and the Nature of the Chemical Bond*.