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## 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*

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## Research Experience

- 2014-Present **PhD. Candidate**, *University of Pittsburgh, Department of Chemical and Petroleum Engineering*, Pittsburgh, PA.  
**Atomically-precise Nanocluster 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 for catalysis.  
**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**

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## Publications

- [1] M. G. Taylor and G. Mpourmpakis. “Rethinking Heterometal Doping in Ligand-Protected Metal Nanoclusters.” In: *Journal of Physical Chemistry Letters*, **Cover Highlight** 9.23 (2018), pp. 6773–6778. DOI: 10.1021/acs.jpclett.8b02679.
- [2] 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* 18.9 (2018), pp. 1528–7483. DOI: 10.1021/acs.cgd.8b00945.
- [3] 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.

- [4] 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.
- [5] 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 Au<sub>24</sub>(SR)<sub>20</sub> nanocluster by silver”. In: *Journal of Colloid and Interface Science* 505 (2017), pp. 1202–1207. DOI: 10.1016/j.jcis.2017.06.049.
- [6] M. G. Taylor and G. Mpourmpakis. “Thermodynamic Stability of Ligand-Protected Metal Nanoclusters”. In: *Nature Communications* 8 (2017), p. 15988. DOI: 10.1038/ncomms15988.
- [7] 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.
- [8] 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.
- [9] 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.
- [10] 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, \$250.
- Dec. 2018 **Dr. James M. Coull Memorial Fellowship Award (highest honor for a graduate student as "most productive")**, Department of Chemical and Petroleum Engineering University of Pittsburgh, \$1500.
- Dec. 2017 **Led: Extreme Science and Engineering Discovery Environment (XSEDE) Proposal**, National Science Foundation (NSF), \$32,355.54.
- Apr. 2015 **GRFP - Honorable Mention**, NSF.
- Apr. 2019 **ChE Outstanding Research Assistant Award**, Engineering Graduate Student Organization, University of Pittsburgh.
- 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. 2018 **XSEDE Proposal (Contributed)**, NSF, \$33,370.34.
- 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.
- [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.*

3700 O'Hara Street, 940 Benedum Hall – Pittsburgh, PA 15213

✉ [mgt16@pitt.edu](mailto:mgt16@pitt.edu) • 🌐 [mgt16.github.io](https://github.com/mgt16)

**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.

Mar. 2019 **Covestro Pittsburgh Regional Science & Engineering Fair**, Pittsburgh, PA.

Served as an awards judge for the Intermediate Chemistry division.

Feb. 2019 **Engineer the Future**, Carnegie Science Center.

Gave Chemical Engineering career advice to senior high school students. Demonstrated basic phase change experiments to the public.

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

Served on the editorial board as a reviewer for Ingenium, the School of Engineering undergraduate research publication.

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

Presented an informative and motivational talk on personal experiences as a Chemical Engineer and scientist to a high school, pre-engineering class (around 50 students).

Apr. 2016 **Undergraduate research seminar presentation**, University of Pittsburgh, Department of Chemical Engineering.

Presented personal research and experiences in graduate school to undergraduates in the department advising them on their future careers.

Apr. 2015 **ISEF**, Pittsburgh, PA.

Served as volunteer for safety and initial inspection of posters at the international high-school science fair.

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## 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)

March 2019 **CHE 2101 - Graduate Chemical Engineering Thermodynamics**, University of Pittsburgh, 20 Students.

Gave 40 minute lecture on my published research highlighting connections to thermodynamics.

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.

Advised several students individually on future career directions and graduate school applications.

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## Professional Society Memberships

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

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

2013-Present **Tau Beta Pi Engineering Honors Fraternity (TBP).**

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## Computational Expertise

Languages Proficient in: Python, BASH, ASE package, R, MATLAB, Some experience in FORTRAN  
Modeling CP<sub>2</sub>K (Molecular and Periodic DFT), Turbomole, LAMMPS, DFTB+, Gaussian  
Platforms GNU/Linux (Redhat/Ubuntu), MacOS, Windows  
Typesetting L<sup>A</sup>T<sub>E</sub>X, Markdown, Word  
Web Github Pages/Jekyll  
Visualization Blender, GIMP, Origin, Inkscape, Matplotlib  
Development git, vim

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## 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.*

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## References

Available Upon Request..