Giannis Mpourmpakis (Ioannis Bourmpakis), PhD

Bicentennial Alumni Faculty Fellow, Assistant Professor,
Department of Chemical and Petroleum Engineering, University of Pittsburgh
905 Benedum Hall, 3700 O'Hara Street, Pittsburgh, PA 15261, USA
Phone: (001) 412-624-7034
Email: gmpourmp@pitt.edu, Website: www.mpourmpakis.com

EDUCATION

Ph.D. in Theoretical and Computational Chemistry (2006)
Chemistry Department, University of Crete, Greece.
Dissertation: "Hydrogen Storage in Nanomaterials".
Advisor: Prof. George E. Froudakis, Chemistry Department, University of Crete.

M.S. in Applied Molecular Spectroscopy (2003)
Chemistry Department, University of Crete, Greece.
Thesis: "Stabilization of Silicon Nanotubes by Encapsulation of Transition Metal Chains".
Thesis Advisors: Prof. George E. Froudakis, Chemistry Department, University of Crete and Dr. Antonis N. Andriotis, Research Director Foundation for Research and Technology Hellas.

B.S. in Chemistry (2001)
Chemistry Department, University of Crete, Greece.

CURRENT ACADEMIC APPOINTMENT

Bicentennial Alumni Faculty Fellow in Engineering (2017-present)
Assistant Professor (2013-present)
Department of Chemical and Petroleum Engineering, University of Pittsburgh, USA

PRIOR RESEARCH POSITIONS

Senior Researcher (2011-2013)
Catalysis Center for Energy Innovation (CCEI), Energy Frontier Research Center, University of Delaware, USA
co-Principal Investigator on Project: Biomass Conversion to Fuels and Chemicals

Post-Doctoral "Marie-Curie" Research Fellow (2008-2011)
i) 2008-2010 outgoing phase: Center for Catalytic Science and Technology (CCST), Chemical Engineering Department, University of Delaware, USA,
Group Leader: Prof. Dionisios G. Vlachos
ii) 2010-2011 return phase: Institute of Electronic Structure and Laser, Foundation for Research and Technology Hellas, Greece,
Group Leader: Dr. Antonis N. Andriotis
Project: CO Oxidation on Au

Post-Doctoral Researcher **(2006-2008)**
Chemical Engineering Department, University of Delaware, USA
Group Leader: Prof. Dionisios G. Vlachos
Project: Metal Nanoparticle Growth

Visiting Research Student **(2001)**
Institute of Physical and Theoretical Chemistry University of Bonn, Germany,
Group Leader: Prof. Sigrid D. Peyerimhoff
Project: Electronic Spectrum of Linear Hydrocarbons

RESEARCH EXPERIENCE/INTERESTS

Our research expertise is interdisciplinary, blending concepts and techniques from Chemistry, Physics, Materials Science and Chemical Engineering. We use theory and computation to investigate the physicochemical properties of nanomaterials with potential applications in diverse nanotechnological areas, ranging from energy generation and storage, to materials design and catalysis.

Research Thrusts:

a) **Hydrogen Storage** (prior research activity)
We provided a firm understanding on how the structural (curvature and chirality) and electronic (point charges) characteristics of SiC, BN and alkali doped C nanotubes affect the physisorption of molecular hydrogen. Based on this, we proposed strategies to design novel nanomaterials exhibiting increased hydrogen storage behavior.

b) **Nanomaterials Growth**
We investigate the colloidal nanoparticle growth in the presence of solvents and capping agents (ligands). We provide insights into the nanoparticle growth mechanisms and propose design guidelines to control nanoparticle characteristics (size, shape, dispersity) during synthesis. We focus on pure and metal-doped, atomically precise thiolate-protected Au nanoclusters, while knowledge gained from nanoparticle growth is also applied to understanding the mechanisms of inhibiting kidney stone growth.

c) **Nanocatalysis**
We elucidate the bonding characteristics of adsorbates on nanoparticles and develop relationships predicting their binding energy versus the nanoparticle structural characteristics (size, shape, metal composition). Additionally, we investigate the catalytic mechanisms on both metals and metal oxide supports by taking into account complex physical phenomena (support effects and reconstruction) occurring on the catalyst. Finally, we propose novel nanocatalysts with optimal catalytic activity under experimental conditions. Reactions of interest include the low-temperature CO oxidation and CO_2 reduction.

d) **Metal-Oxide Chemistry**
We investigate catalytic reactions relevant to the production of olefins from biomass (e.g. alcohols) and petrochemical sources (e.g. alkanes) on various metal-oxides. We develop structure-activity relationships as a function of the metal-oxide acid-base properties and the reactants substitution, aiming to screen different oxides with respect to their catalytic activity and selectivity to desired products.

PUBLICATIONS IN REFEREED JOURNALS

(H-INDEX=25, CITATIONS=2461 (GOOGLE SCHOLAR 09/29/2018); H-INDEX=23, CITATIONS=1987 (SCOPUS, 09/29/2018))

Peer-reviewed publications at Pitt:

Manuscripts in preparation

81. Solvent Manipulation of the Pre-reduction Metal-Ligand Complex for Controlled Growth of Pd Nanoparticles
Li W., Taylor M.G., Mozaffari S., Ivanov S., Seifert S., Lee B., Shanaiah N., Lu Y., Kovarik L., Mpourmpakis G., Karim A.M.
under preparation for submission to *J. Amer. Chem. Soc.* (2018)

80. Universal Adsorption Models on Metal Nanoparticles: Connecting Stability with Catalysis
Taylor M.G., Dean J.R., Yan Z. and Mpourmpakis G.
under preparation for submission to *Science Advances* (2018)

79. Elucidating the Role of Water in Alcohol Dehydration on γ-Al_2O_3 using First-Principles-Based Microkinetic Modeling
Tancini P., Kostetskyy P., Kaisare N., Maestri M., Mpourmpakis G.
under preparation for submission to *Applied Catalysis A* (2018)

Manuscripts under review

78. Computational Study of Methane Activation on γ-Al_2O_3
Cholewinski M., Dixit M. and Mpourmpakis G.
under in *ACS Omega* (2018)

77. Structure-property Relationships on Thiolate-protected Gold Nanoclusters
Cowan M. and Mpourmpakis G.
under review in *RSC Nanoscale Advances* (2018)

76. Understanding Alkane Dehydrogenation through Alcohol Dehydration on γ-Al_2O_3
Kostetskyy P., Nolan C., Dixit M., Mpourmpakis G.
under review in *Industrial & Engineering Chemistry Research* (2018)

Manuscripts under revision

75. Rethinking Heterometal Doping in Ligand-Protected Metal Nanoclusters
Taylor M.G. and Mpourmpakis G.
under minor revision in *Journal of Physical Chemistry Letters* (2018)

74. Structure Activity Relationships in Alkane Dehydrogenation on γ-Al_2O_3: Site-Dependent Reactions
Dixit M., Kostetskyy P., Mpourmpakis G.
under revision in *ACS Catalysis* (2018)

Published journal articles

73. Elucidating the active sites for CO_2 electroreduction on ligand-protected Au_{25} nanoclusters
Austin N., Zhao S., McKone J.R., Jin R., Mpourmpakis G.
Catal. Sci. & Technol. 8, 3795-3805 (2018)

72. Factors Differentiating the Effectiveness of Polyprotic Acids as Inhibitors of Calcium Oxalate Crystallization in Kidney Stone Disease
Chung J., Taylor M., Granja I., Asplin J., Mpourmpakis G., Rimer J.
Journal of Crystal Growth & Design 18, 5617–5627 (2018)

71. Understanding the Gas Phase Chemistry of Alkanes with First-Principles Calculations
Estes J.E., Dixit M., Mpourmpakis G.
J. Chem. Eng. Data 63, 2430–2437 (2018) **Invited contribution as an "Emerging Investigator" (2018)**

70. Size, Shape and Composition Dependent Model for Metal Nanoparticle Stability Prediction, Yan Z., Taylor M., Mascareno A., Mpourmpakis G.
Nano Lett. 18, 2696–2704, (2018)
69. Influence of Atomic-level Morphology on Catalysis: The Case of Sphere and Rod-like Gold Nanoclusters for CO_2 Electroreduction
Zhao S., Austin N., Li M., Song Y., House S.D., Bernhard S., Yang J.C., Mpourmpakis G., Jin R.
ACS Catal. 8, 4996-5001 (2018)
67. Design of Copper-Based Bimetallic Nanoparticles for Carbon Dioxide Adsorption and Activation
Dean J., Yang Y., Austin N., Veser G. Mpourmpakis G.
ChemSusChem 11, 1169 –1178 (2018) **journal cover of issue 7**
66. Design of Highly Selective Ethanol Dehydration Nanocatalysts for Ethylene Production
Austin N., Kostetskyy P., Mpourmpakis G.
Nanoscale 10, 4004 – 4009 (2018)
65. Direct Catalytic Conversion of Biomass-Derived Furan and Ethanol to Ethylbenzene
Teixeira I.F., Lo B.T.W., Kostetskyy P., Ye L., Tang C.C., Mpourmpakis G., Tsang E.C.S.
ACS Catalysis 8, 1843–1850 (2018)
64. Mechanistic studies on the Michael addition of amines and hydrazines to nitrostyrenes: Nitroalkane elimination via a retro-aza-Henry type process
Kallitsakis M., Tancini P., Dixit M., Mpourmpakis G., Lykakis I.
J. Org. Chem. 83, 1176-1184 (2018)
63. Reconstructing the Surface of Gold Nanocluster by Cadmium Doping
Li Q., Lambright K.J., Taylor M.G., Kirschbaum K., Luo TY, Zhao J., Mpourmpakis G., Mokashi-Punekar S., Rosi N.L., Jin R.
J. Amer. Chem. Soc. 139, 17779–17782 (2017)
62. Elucidating the Role of Oxygen Coverage in CO_2 Reduction on Mo_2C
Dixit M., Peng X., Porosoff M.D., Willauer H.D. Mpourmpakis G.
Catal. Sci. & Technol. 7, 5521-5529 (2017) **journal cover of issue 23 and selected as hot article for 2017**
61. Thermodynamic Stability of Ligand-Protected Metal Nanoclusters
Taylor M. and Mpourmpakis G.,
Nature Communications 8, 15988 (2017)
Article metrics: https://www.nature.com/articles/ncomms15988/metrics
Commentary by NanoToday Editor:
https://www.materialstoday.com/nanomaterials/news/researchers-unlock-key-to-nanocluster-formation/
60. Site-selective Substitution of Gold Atoms in the $Au_{24}(SR)_{20}$ Nanocluster by Silver
Li Q., Taylor M.G., Kirschbaum K., Lambright K., Zhu X. Mpourmpakis G., Jin R.
Journal of Colloid and Interface Science, 505, 1202-1207, (2017)
59. Computational Insights into Adsorption of C4 Hydrocarbons in Cation-Exchanged ZSM-12 Zeolites
Kostetskyy P. and Mpourmpakis G.
Industrial & Engineering Chemistry Research, 56, 7062–7069, (2017) **journal cover of issue 26**
58. Molecular "surgery" on a 23-gold-atom nanoparticle
Li Q., Luo T.-Y., Taylor M.G., Wang S., Zhu X., Song Y., Mpourmpakis G., Rosi N.L., Jin R.,
Science Advances 3, e1603193 (2017)
57. Potassium-promoted molybdenum carbide as a highly active and selective catalyst for CO_2 conversion to CO
Porosoff M.D., Baldwin J.W., Peng X., Mpourmpakis G., Willauer H.D.
ChemSusChem 10, 2408 –2415 (2017) **journal cover of issue 10**

56. CO_2 Activation on Cu-based Zr-Decorated Nanoparticles
Austin N., Ye J. and Mpourmpakis G.
Catal. Sci. & Technol. 7, 2245-2251 (2017)
55. Carboranes: The Strongest Brønsted Acids in Alcohol Dehydration
Kostetskyy P., Zervoudis N.A. and Mpourmpakis G.
Catal. Sci. & Technol. 7, 2001-2011 (2017) **journal cover of issue 8 and selected as hot article for 2017**
54. CO_2 Activation on Bimetallic CuNi Nanoparticles
Austin N., Butina B. and Mpourmpakis G.
Invited Article on Themed Issue on Nanomaterials in *Progress in Natural Science: Materials International* 26, 487–492 (2016)
53. Molecular modifiers reveal a mechanism of pathological crystal growth inhibition
Chung J., Granja I., Taylor M., Mpourmpakis G., Asplin J., Rimer J.
Nature 536, 446–450 (2016)
Highlighted in 77 news outlets across the world:
http://www.nature.com/nature/journal/v536/n7617/nature19062/metrics/index.html
52. From Biomass-Derived Furans to Aromatics with Ethanol over Zeolite
Teixeira I.F., Lo B.T.W., Kostetskyy P., Stamatakis M., Ye L., Tang C.C., Mpourmpakis G., Tsang E.C.S.
Angewandte Chemie Int. Ed. 55 (42), 13061–13066 (2016), **journal cover of issue 42**
51. Description and Role of Bimetallic Pre-nucleation Species in the Formation of Small Nanoparticle Alloys
Marbella L.E., Chevrier D.M., Tancini P.D., Shobayo O., Smith A.M., Johnston K.A., Andolina C.M., Zhang P., Mpourmpakis G., Millstone J.E.
J. Amer. Chem. Soc. 137, 15852–15858 (2015)
50. Catalyst Design Based on Morphology- and Environment-Dependent Adsorption on Metal Nanoparticles
Taylor M.G., Austin N., Gounaris C., Mpourmpakis G.
ACS Catal. 5, 6296–6301 (2015)
49. Structure-activity relationships in the production of olefins from alcohols and ethers: A first-principles theoretical study
Kostetskyy P. and Mpourmpakis G.,
Catal. Sci. & Technol., 5, 4547 – 4555 (2015)
48. Au_{13}: CO Adsorbs, Nanoparticle Responds.
Austin N., Johnson J.K. and Mpourmpakis G.
J. Phys. Chem. C 119, 18196–18202 (2015), **journal cover of issue 32**
47. Understanding the importance of carbenium ions in the conversion of biomass-derived alcohols with first principles calculations
Kostetskyy P., Maheswari J.P., Mpourmpakis G.,
J. Phys. Chem. C 119, 16139–16147 (2015)
46. Catalysis at the Sub-Nanoscale: Complex CO Oxidation Chemistry on a Few Au Atoms
Nikbin N., Austin N., Vlachos D.G., Stamatakis M., Mpourmpakis G.
Catal. Sci. & Technol. 5, 134–141 (2015), **journal cover of issue 1**
Featured in: https://ichemepresident.wordpress.com/2014/12/23/a-precious-catalyst-day-210/#more-5407
45. DFT-driven Multi-Site Microkinetic Modeling of Ethanol Conversion to Ethylene and Diethyl Ether on γ-Al_2O_3(111)
Christiansen M.A., Mpourmpakis G. and Vlachos D.G.
J. Catalysis 323, 121-131 (2015), **featured article**
44. Understanding the Stability, Electronic, and Adsorption Properties of Sub-nanometer Group XI Monometallic and Bimetallic Catalysts

Austin N. and Mpourmpakis G.
J. Phys. Chem. C 118, 18521−18528 (2014)
43. Structure-Activity Relationships on Metal-Oxides: Alcohol Dehydration
Kostestkyy P., Yu J., Gorte R.J. and Mpourmpakis G.
Catal. Sci. & Technol. 4, 3861–3869 (2014) **journal cover of issue 11**
42. Informatics Guided Discovery of Surface Structure-Chemistry Relationships in Catalytic Nanoparticles
Andriotis A.N., Mpourmpakis G., Broderick S., Rajan K., Datta S., Sunkara M., and Menon M.
J. Chem. Phys. 140, 094705 (2014)

Peer-reviewed publications prior to Pitt (as senior researcher and post-doc):
41. Adsorption behavior of noble metal clusters and their alloys
Herrmann S., Stamatakis M., Andriotis A.N. and Mpourmpakis G.
J. Comput. Theor. Nanosci. 11, 511-520 (2014)
40. Determination of Proton Affinities and Acidity Constants of Sugars
Feng S., Bagia C. and Mpourmpakis G.
J. Phys. Chem. A 117, 5211-5219 (2013)
39. DFT-Computed Mechanisms of Ethylene and Diethyl Ether Formation from Ethanol on γ-Al_2O_3(100)
Christiansen M., Mpourmpakis G. and Vlachos D.G.
ACS Catal. 3, 1965–1975, (2013)
38. Effect of Oxide Supports in Stabilizing Desirable Pt–Ni Bimetallic Structures for Hydrogenation and Reforming Reactions
Wang T., Mpourmpakis G., Lonergan W.W., Porosoff M.D., Vlachos D.G., Chen J.G.,
*Phys. Chem. Chem. Phys.*15, 12156-12164 (2013)
37. U-calculation of the LSDA plus U functional using the hybrid B3LYP and HSE functionals
Andriotis A.N., Mpourmpakis G., Lisenkov S., Sheetz R.M. and Menon M.
Phys. Status Solidi (b) 250, 356-363, (2013)
36. A DFT study of furfural conversion to furan, furfuryl alcohol, and 2-methylfuran on Pd(111)
Vorotnikov V., Mpourmpakis G. and Vlachos D.G.
ACS Catal. 2, 2496−2504 (2012)
35. Liquid-Phase Dehydration of Propylene Glycol Using Solid-Acid Catalysts
Courtney T.D., Nikolakis V., Mpourmpakis G., Chen J.G. and Vlachos D.G.
Appl. Catal. A 449, 59– 68 (2012)
34. A Mechanistic Study of Alcohol Dehydration on γ-Al_2O_3
Roy S., Mpourmpakis G., Hong D.-Y., Vlachos D.G., Bhan A. And Gorte R.J.
ACS Catal. 2, 1846−1853 (2012)
33. Multiscale Modeling Reveals Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation
Stamatakis M., Christiansen M., Vlachos D.G. and Mpourmpakis G.
Nano Lett. 12, 3621–3626 (2012)
32. A Combined DFT and Statistical Mechanics Study for the CO Oxidation on the Au_{10}^{-1} cluster.
Nikbin N., Mpourmpakis G. and Vlachos D.G.
J. Phys. Chem. C 115, 20192–20200 (2011)
31. Predicting the Adsorption Behavior in Bulk from Metal Clusters
Mpourmpakis G., Stamatakis M., Herrmann S., Vlachos D.G. and Andriotis A.N.
Chem. Phys. Lett. 518, 99-103 (2011)
30. Symmetry-switching molecular $Fe(O_2)_n^+$ clusters
Mpourmpakis G., Velegrakis M., Mihesan C. and Andriotis A.N.
J. Phys. Chem. A 115, 26, 7456-7460 (2011)
29. Computational-Based Catalyst Design for Thermochemical Transformations

Mpourmpakis G. and Vlachos D.G.
MRS Bulletin 36, 211-215 (2011)
28. What Controls Au Nanoparticle Dispersity during Growth?
Mpourmpakis G., Caratzoulas S. And Vlachos D.G.
Nano Lett. 10, 3408-3413 (2010)
27. Identification of Descriptors for the CO Interaction with Metal Nanoparticles
Mpourmpakis G., Andriotis A.N. and Vlachos D.G.
Nano Lett. 10, 1041-1045 (2010)
26. Correlating Particle Size and Shape of Supported Ru/g-Al_2O_3 catalysts with NH_3 Decomposition Activity
Karim A., Prasad V., Mpourmpakis G., Lonergan W., Frenkel A., Chen J., Vlachos D.G.
J. Amer. Chem. Soc., 131, 12230-12239 (2009)
25. The Effects of the MgO Support and Alkali Doping on the CO Interaction with Au
Mpourmpakis G. and Vlachos D.G.
J. Phys. Chem. C, 113, 7329–7335 (2009)
24. Growth Mechanisms of Metal Nanoparticles via First Principles
Mpourmpakis G. and Vlachos D.G.
Phys. Rev. Lett. 102, 155505 (2009)
23. Insights into the Early Stages of Metal Nanoparticle Formation via First Principle Calculations: The Roles of Citrate and Water.
Mpourmpakis G. and Vlachos D.G.
Langmuir 24, 7465-7473 (2008)
22. Surface Conductivity of Hydrogenated Diamond Films.
Andriotis A.N., Mpourmpakis G., Richter E., Menon M.
Phys. Rev. Lett. 100**,** 106801 (2008)

Peer-reviewed publications from PhD, MS and BS:
21. Assessing the Density Functional Theory in the Hydrogen Storage problem.
Mpourmpakis G. and Froudakis G.E.
J. Nanosci. Nanotechnol. 8, 3091–3096 (2008)
20. Carbon Nanoscrolls: A Promising Material for Hydrogen Storage Applications.
Mpourmpakis G., Tylianakis E., Froudakis G.E.
Nano Lett. **7**, 1893-1897 (2007)
Appears also in: NewScientistTech: Roll up for better hydrogen fuel storage
https://www.newscientist.com/article/dn12128-roll-up-for-better-hydrogen-fuel-storage/
19. Enhancement of the Ionization-Potential of K and Rb upon Chemisorption on a C60 Molecule.
Mpourmpakis G., Froudakis G.E., Andriotis A.N., Menon M.
J. Phys. Chem. C 111, 6593-6596 (2007)
18. The Effect of Curvature and Chirality for Hydrogen Storage in SWNTs. A Combined *Ab-initio* and Monte-Carlo Investigation.
Mpourmpakis G., Froudakis G.E., Lithoxoos G.P., Samios J.
J. Chem. Phys. 126, 144704 (2007)
17. Why Boron Nitride Nanotubes are Preferable to Carbon Nanotubes for Hydrogen Storage? An *ab-initio* Theoretical Study
Mpourmpakis G. and Froudakis G.E.
Catal. Today 120, 341-345 (2007)
16. Haeckelites: A New Promising Anode Material for Lithium Batteries Application. A Multi Scale Theoretical Study.
Mpourmpakis G., Tylianakis E., Froudakis G.E.
Appl. Phys. Let. 89, 233125 (2006)

15. Why Alkali Metals Preferably Bind on Structural Defects of Carbon Nanotubes.
A Theoretical Study by First Principles.
Mpourmpakis G. and Froudakis G.E.
J. Chem. Phys. 125, 204707 (2006)
14. SiC Nanotubes: A Novel Material for Hydrogen Storage Applications.
Mpourmpakis G., Froudakis G.E., Lithoxoos G.P., Samios J.
Nano Lett. 6, 1581-1583 (2006) most accessed article in the period July-September 2006
13. Multi Scale Theoretical Study of Li^+ Interaction with Carbon Nanotubes
Mpourmpakis G, Tylianakis E, Papanikolaou D, Froudakis G
J. Nanosci. Nanotechnol. 6, 3731-3735 (2006)
12. Theoretical Study of Alkaline Metal Cations in Carbon Nanotubes
Mpourmpakis G, Tylianakis E, Papanikolaou D, Froudakis G
Rev. Adv. Mat. Sci. 11, 92 (2006)
11. Hydrogen Storage in Carbon Nanotubes: A Multi-Scale Theoretical Study
Mpourmpakis G., Tylianakis E., Froudakis G.E.
J. Nanosci. Nanotechnol. 6, 87-90 (2006)
10. Carbon-nanotube tips with edge made of a transition metal
Mpourmpakis G., Froudakis G.E., Andriotis A.N., Menon M.
Appl. Phys. Lett. 87, 193105 (2005)
9. Role of Co in Enhancing the Magnetism of Small Fe Clusters
Mpourmpakis G., Froudakis G.E., Andriotis A.N., Menon M.
Phys. Rev. B 72, 104417 (2005)
8. State-Specific RKKY Interaction in Small Magnetic Clusters
Andriotis A.N., Mpourmpakis G., Froudakis G.E., Menon M.
Phys. Rev. B 70, 104421 (2004)
7. Magnetic Enhancement and Magnetic Reduction in Binary Clusters of Transition Metal Atoms
Andriotis A.N., Mpourmpakis G., Froudakis G.E., Menon M.
J. Chem. Phys. 120, 11901 (2004)
6. Fe Encapsulation by Silicon Clusters: Ab initio Electronic Structure Calculations
Mpourmpakis G., Froudakis G.E., Andriotis A.N., Menon M.
Phys. Rev. B 68, 125407 (2003)
5. Understanding the Structure of Metal Encapsulated Si Cages and Nanotubes: Role of Symmetry and d-band Filling
Mpourmpakis G., Froudakis G.E., Andriotis A.N., Menon M.
J. Chem. Phys. 119, 7498 (2003)
4. Ab initio MRD-CI Investigation of Linear HC_5H^+ and HC_7H^+ .
Mühlhäuser M., Haubrich J., Mpourmpakis G., Mavrandonakis A., Froudakis G.E.
Internet Electronic Journal of Molecular Design, **2** biochemm press, (2003)
3. Ene Hydroperoxidation of Isobutenylarenes within Dye-Exchanged Zeolite Na-Y: Control of Site Selectivity by Cation-Arene Interactions
Stratakis M., Rabalakos C., Mpourmpakis G., Froudakis G.E.
J. Org. Chem. 68, 2839 (2003)
2. Stabilization of Si-based Cage Clusters and Nanotubes by Encapsulation of Transition Metal Atoms
Andriotis A.N., Mpourmpakis G., Froudakis G.E., Menon M.
New J. Phys. 4, 78 (2002)
1. Importance of Multi-Reference Configuration Interaction for $^3\Sigma_u^- \leftarrow X^3\Sigma_u^-$ Transitions of Linear HC_7H
Mpourmpakis G., Muhlhauser M., Froudakis G.E., Peyerimhoff S.D.
Chem. Phys. Lett. 356, 398-402 (2002)

PATENTS

Patent Title: Reactive Extraction of Water
Application No.: 62/470,664,
Innovators: Eric J. Beckman and Ioannis Bourmpakis (University of Pittsburgh)
Status: Filed

BOOK CHAPTERS

4. Chapter in Book: "Chemistry of Carbon Nanotubes" (V.A. Basiuk and E.V. Basiuk, Eds.) by American Scientific Publishers, Title: Interaction of hydrogen with carbon Nanotubes, G. Mpourmpakis, E. Tylianakis, G. E. Froudakis,
3. Laboratory Exercises of Physics, Technological Educational Institute of Crete, School of Health and Social Welfare, Department of Human Nutrition and Dietetics. (in Greek)
Authors: Fthenakis Zaharias and Mpourmpakis Giannis.
2. "Theoretical Investigation of Hydrogen Storage in Nanomaterials" Chemistry Department, University of Crete (Phd thesis, in Greek)
1. "Stabilization of Silicon Nanotubes by Encapsulation of Transition Metal Chains" Chemistry Department, University of Crete and Foundation for Research and Technology Hellas (MS thesis, in Greek)

PARTICIPATION IN CONFERENCES/PRESENTATIONS

Invited Talks/Seminars:

- Department of Chemical Engineering, University of Rochester, NY, USA, scheduled for September 2019
  "Designing Nanocatalysts for CO_2 Reduction"
- Braskem, Pittsburgh PA, USA, May 29, 2018
  "Developing Structure-Activity Relationships for Ethylene Production Chemistries"
- Department of Chemistry, University of California Los Angeles, CA, May 21, 2018
  "Insights into the Stability and Catalysis of Ligand-Protected Nanoclusters"
- Department of Chemistry, University of Colorado, Denver CO, USA, May 4 2018
  "Understanding the Stability and Catalytic Behavior of Ligand-Protected Nanoclusters with Computational Modeling"
- New York Catalysis Society Annual Meeting, Bethlehem PA, USA, March 26 2018
  "How Structure Affects Stability and Catalysis of Metal Nanoparticles"
- Department of Chemical Engineering, Virginia Tech University, Blacksburg VA, USA, September 15, 2017, "Understanding Au Nanoparticle Formation and Catalysis with Computational Modeling"
- National Energy and Technology Laboratory, Pittsburgh PA, USA, August 9, 2017
  "Computational Design of Active Nanocatalysts"
- Southwest Catalysis Society, 2017 Symposium, Houston TX., USA, April 28, 2017
  "Computational Design of Catalytic Nanoparticles"
- 2016 ACS National Meeting, Advances in Computational Catalysis Symposium, Philadelphia, PA, USA, August 21-25, 2016, "Adsorption on Metal Nanoparticles: Effects from Size, Shape and Chemical Environment"
- 2015 Lubrizol University Contacts Meeting, Brecksville OH, USA, August 26, 2015
  "Viscosity Creep in Lubrizol Additives: Mechanistic Insights from First Principles Calculations"
- Lubrizol Wickliffe OH, USA, January 22, 2015
  "In-Silico Catalyst Design"
- Department of Chemistry, University of Pittsburgh, Pittsburgh PA, USA, December 11, 2014, "In-Silico Catalyst Design"

- Pittsburgh Cleveland Catalysis Society meeting, Pittsburgh PA, USA June 2, 2014
  "Catalytic Complexity in Simple Reactions: Insights from First Principles Calculations"
- Department of Materials Science and Engineering, University of Michigan, Ann Arbor MI, USA, April 18, 2014
  "Understanding the Complexity in Catalyst Design through First Principles Calculations".
- Braskem, Pittsburgh PA, USA, Nov. 26 2013 (broadcast to Brazil)
  "Understanding Dehydration in Biomass Conversion to Value-Added Chemicals"

Prior to Pitt:
- Chemistry Department, University of Athens, Greece, December 2010
  "Growth Mechanisms of Metal Nanoparticles using Computational Methods"
- Chemistry Department, University of Crete, Greece, May 7, 2010
  "Multiscale Simulations of Gold Catalysis"
- 2012 CCST Research Review: October 4, 2012, University of Delaware, USA
  "Alcohol Dehydration Chemistry"

Presentations/Contributions:
(Presenting author underlined)

- 2018 AIChE National Meeting, Pittsburgh PA, Oct. 28 – Nov. 2, 2018
  Talk: "CO_2 Reduction on Ligand-Protected Au Nanoclusters"
  Mpourmpakis G. and Austin N.
  Talk: "Development of a Bond-Centric Model for Thermodynamic Stability of Nanoalloys"
  Taylor M.G., Yan Z., Mascareno A. and Mpourmpakis G.,
  Talk: "Rationalizing Stability and Doping of Atomically Precise Ligand-Protected Metal Nanoclusters"
  Taylor M.G., Li Q., Jin R. and Mpourmpakis G
  Talk: "Computational Study of Methane Activation on γ-Al_2O_3"
  Dixit M., Cholewinski M. and Mpourmpakis G.
  Talk: "Computational Prediction of the Structure and Catalytic Properties of Copper Zirconium Oxide"
  Dean J. and Mpourmpakis G.
  Talk: "Identification of Optimally Stable Nanoparticle Geometries Via Mathematical Optimization and Density-Functional Theory"
  Isenberg N.M., Yan Z., Taylor M.G., Hanselman C., Mpourmpakis G. and Gounaris C.E.
  Talk: "Elucidating the Role of Oxygen Coverage in CO_2 Reduction on Mo_2C"
  Dixit M., Peng X., Porosoff M.D., Mpourmpakis G. and Willauer H.D.
  Poster: "Computer-Aided Description of Materials Stability at the Nanoscale"
  Taylor M.G. and Mpourmpakis G.
  Poster: "Thermodynamic Stability of Thiolate-Protected Gold Nanoclusters: From Molecular to Metallic Systems"
  Cowan M., Taylor M.G. and Mpourmpakis G.
- 2018 ACS National Meeting, New Orleans LA, Mar. 18 – Mar. 22, 2018
  Talk: "Elucidating the role of oxygen coverage in CO_2 reduction on Mo_2C"
  Dixit M., Peng Xi, Porosoff M. D., Willauer H. D. and Mpourmpakis G.
- 2017 AIChE National Meeting, Minneapolis MN, Oct. 28 – Nov. 3, 2017
  Talk: "Computational design of thermodynamic stable metal nanoparticles"
  Mpourmpakis G.
  Talk: "Structure-activity relations on γ-Al_2O_3: From alcohol dehydration to alkane dehydrogenation"

Kostetskyy P. and Mpourmpakis G.
Talk: "Understanding the C-H activation mechanisms of alkanes on metal oxides"
Dixit M. and Mpourmpakis G.
Talk: "Designing Cu-based bimetallic nanoparticles for CO_2 activation"
Dean J. and Mpourmpakis G.
Talk: "Colloidal Pd Nanoparticle Synthesis: The Effect of Ligand-Metal-Solvent Thermodynamics on Kinetics and Final Size"
Li W., Wooten C., Ivanov S.A., Mozaffari S., Taylor M.G., Mpourmpakis G. and Karim A.M.

- 2017 ACS National Meeting, Washington DC, August 20-25, 2017
  Talk: "Engineering ligand-protected Au nanoclusters for CO_2 reduction"
  Austin N. and Mpourmpakis G.
  Talk: "Developing structure activity relationships in the dehydrogenation of alkanes on oxides"
  Dixit M. and Mpourmpakis G.
- 2017 Pittsburgh Simulators Meeting, Carnegie Mellon University, Pittsburgh PA, USA, May 31, 2017.
  Talk: "Designing Cu-based Bimetallic Nanoparticles for CO_2 Activation"
  Dean J. and Mpourmpakis G.
- Pittsburgh-Cleveland Catalysis Society Annual Meeting (2017), Akron OH, USA, May 25, 2017
  Poster: "Understanding the C-H Activation and Dehydrogenation Mechanisms of Alkanes on γ-Alumina"
  Dixit M. and Mpourmpakis, G.
  Poster: "CO_2 Activation on Cu-based Bimetallic Nanoparticles"
  Dean J., Austin N., and Mpourmpakis G.
- Advancing Research Through Computing Conference, Pittsburgh, PA, Mar. 2, 2017
  Poster: "Stability and Prediction of Thiolated Metal Nanoclusters"
  Taylor M.G. and Mpourmpakis G.
- AIChE 2016 National Meeting, San Francisco CA, USA, Nov. 13 – Nov. 18, 2016
  Talk: "CO_2 Activation on Zr-Decorated, Cu Nanoparticles"
  Austin N. and Mpourmpakis G.
  Talk: "Computational Insights into DMF Conversion to p-Xylene: Ethylene or Ethanol?"
  Kostetskyy P., Teixeira I., Stamatakis M., Tsang S.C.E. and Mpourmpakis G.
  Talk: "Structure-Dependent Stability of Magic-Number Thiolated Metal Nanoparticles"
  Taylor, M. G. and Mpourmpakis G.
  Poster: "Understanding Water Effects in Alcohol Dehydration Activity on γ-Al_2O_3 Using Microkinetic Modeling"
  Tancini P., Kostetskyy P., Kaisare N., Maestri M. and Mpourmpakis G.
- Pittsburgh Cleveland Catalysis Society Annual Meeting, Pittsburgh PA, USA, Sept. 23, 2016
  Talk: "Computational Insights into DMF Conversion to p-Xylene: Ethylene or Ethanol?"
  Kostetskyy P., Teixeira I., Stamatakis M., Tsang S.C.E. and Mpourmpakis G.
- ACS 2016 National Meeting, Philadelphia, PA, Aug. 21 – Aug. 25, 2016
  Talk: "Computational design of Zr-decorated, Cu-based Nanoparticles for CO_2 activation"
  Austin N. and Mpourmpakis G.
  Talk: "Computational Insights into DMF Conversion to p-Xylene: Ethylene or Ethanol?"
  Kostetskyy P., Teixeira I., Stamatakis M., Tsang S.C.E. and Mpourmpakis G.
  Talk: "Modeling the structure-dependent stability of thiolated metal nanoparticles"
  Taylor, M. G. and Mpourmpakis G.

- Midwest Theoretical Chemistry Conference - Pittsburgh PA, USA, June 9-11, 2016
  Poster: “Exploring the Structure-Dependent Stability of Thiolated Metal Nanoparticles”
  Taylor, M. G. and Mpourmpakis G.
  Poster: “Computational Insights into DMF Conversion to p-Xylene: Ethylene or Ethanol?”
  Kostetskyy P., Teixeira I., Stamatakis M., Tsang S.C.E. and Mpourmpakis G.
- AIChE 2015 National Meeting, Salt Lake City UT, USA, Nov.8 – Nov. 13, 2015
  Talk: “Kidney Stone Growth Modification: Insights from First Principles Calculations”
  Taylor M. G., Chung J., Carnaval I., Rimer J. D., and Mpourmpakis G.
  Talk: “Inhibition of Calcium Oxalate Monohydrate Crystallization Using Organic Acids”
  Chung J., Taylor M. G., Carnaval I., Mpourmpakis G., Asplin, J. R., and Rimer J. D.
  Talk: “Generalized Dehydration Trends: Connecting Brønsted- with Lewis- Acid Catalysis”
  Kostetskyy P., Zervoudis N. Maheswari J.P. and Mpourmpakis G.
  Poster: “Formation Pathways of Pre-Nucleation Species in AuCu Bimetallic Nanoparticle Growth: A First Principles Study”
  Tancini P., Marbella L.E., Millstone J.E. and Mpourmpakis G.
- Advancing Research through Computing Symposium, Pittsburgh PA, October 29, 2015
  Poster: “Advancing Catalyst Design: Adsorption Models Accounting for Nanoparticle Size, Shape, and Chemical Environment”
  Austin N. and Mpourmpakis G.
  Poster: “Structure-Activity Relationships in Alcohol Dehydration on Metal-Oxides”
  Kostetskyy P. and Mpourmpakis G.
- NAM24, Pittsburgh PA, USA, June 14 – 19, 2015
  Talk: "Adsorbate interactions with metal Nanoparticles"
  Austin N., Taylor M. G., and Mpourmpakis G.
  Poster: "Structure-Activity Relationships in Alcohol Dehydration on Metal-Oxides"
  Kostetskyy P. and Mpourmpakis G.
- 2015 Pittsburgh Simulators Meeting, Carnegie Mellon University, May 18, 2015
  Talk: “Understanding Adsorption at the Nanoscale”
  Austin N., Taylor M. G., and Mpourmpakis G.
  Talk: “Kidney Stone Growth Modification: Insights from First Principles”
  Taylor M. G., Chung J., Carnaval I., Rimer J. D., and Mpourmpakis G.
- AIChE 2014 National Meeting, Atlanta GA, USA, Nov. 16 – Nov. 21, 2014
  Talk: “Adsorption on Metal Nanoparticles: Size and Shape Matters”
  Austin N. and Mpourmpakis G.
  Talk: “Structure-Activity Relationships for the Conversion of Biomass Derived Alcohols to Chemicals”
  Kostetskyy P. and Mpourmpakis G.
  Poster: Understanding the Early Stages of Metal Nanoparticle Growth Using Density Functional Theory Calculations”
  Shobayo O. Millstone J.E. and Mpourmpakis G.
- 2014 Pittsburgh Simulators Meeting, Carnegie Mellon University, June 10, 2014
  Talk: “Understanding the stability, electronic, and adsorption properties of sub-nanometer group XI monometallic and bimetallic catalysts”
  Austin N. and Mpourmpakis G.
- Pittsburgh Cleveland Catalysis Society meeting, Pittsburgh PA, USA June 2, 2014
  Poster: “Structure-Activity Relationships on Metal-Oxides: Alcohol Dehydration”
  Kostetskyy P. and Mpourmpakis G.
  Poster: “Catalyst Design at the Sub-Nanoscale”
  Austin N. and Mpourmpakis G.

- AIChE 2013 National Meeting, San Francisco CA, USA, Nov. 3 – Nov. 8, 2013
  Talk: "Understanding the Alcohol Dehydration on Metal Oxides"
  Mpourmpakis G.

Prior to Pitt:

- AIChE 2012 National Meeting, Pittsburgh PA, USA, Oct. 28 – Nov. 2, 2012
  Talk: "Poisoning Mechanisms of MgO-Supported Au Clusters in CO Oxidation"
  Mpourmpakis G., Stamatakis M., Nikbin N. and Vlachos D.G.
  Talk: "Developing Relationships for the Lewis-Catalyzed Alcohol Dehydration on Alumina"
  Mpourmpakis G. Vlachos D.G. and Gorte R.J.
  poster: "First-Principles Multiscale Modeling of Materials for Energy and Environmental Applications"
  Mpourmpakis G.
- AIChE 2009 National Meeting, Nashville TN, USA, November 8-13, 2009
  Talk: "Charging of metal oxide supported Au clusters and its effect on the CO oxidation reaction"
  Mpourmpakis G. and Vlachos D.G.
- 2009 CCST Research Review: October 8, 2009, University of Delaware, USA
  Talk: "CO Oxidation on Au Nanocatalysts: Insights from First Principles Modeling"
  Mpourmpakis G.
- 21st Meeting of the North American Catalysis Society (21st NAM), San Francisco, USA, June 7-12, 2009 (2 poster presentations)
- 237th ACS National Meeting, Salt Lake City, UT, USA, March 22-26 2009
  Talk: "First principle modeling of catalyst nanoparticle synthesis"
  Mpourmpakis G. and Vlachos D.G.
  Talk: "First principles calculations of supported catalysts: CO binding on MgO supported gold clusters for the CO oxidation reaction"
  Mpourmpakis G. and Vlachos D.G.
- AIChE 2008 National Meeting, Philadelphia PA, USA, November 16-21, 2008
  Talk: "Understanding the silver nanoparticle growth via first principle methods"
  Mpourmpakis G. and Vlachos D.G.
  Talk: "First principle calculations of supported catalysts: CO binding on MgO supported gold clusters and nanoparticles"
  Mpourmpakis G. and Vlachos D.G.
- 2008 CCST Research Review: October 23, 2008, University of Delaware, USA
  Talk: "First principle modeling of catalyst nanoparticle synthesis"
  Mpourmpakis G. and Vlachos D.G.
- 235th ACS National Meeting, New Orleans, LA, USA, April 6-10, 2008
  Talk: "Understanding the silver nanoparticle growth via first principle methods"
  Mpourmpakis G. and Vlachos D.G.
  Talk: "First principle calculations of supported catalysts: CO binding on MgO supported gold clusters and nanoparticles"
  Mpourmpakis G. and Vlachos D.G.
- Fall Research Review '07, Chemical Engineering Department, University of Delaware, USA
  Poster: "First Principles Calculations of Supported Catalysts: CO Binding on MgO Supported Gold Clusters"
  Mpourmpakis G. and Vlachos D.G.
- 2nd Panhellenic Symposium on Porous Materials, National Center of Scientific Research 'Demokritos', Athens, Greece, September 29-30, 2005.

Talk: “Alkali metals interactions with carbon nanotubes”
Mpourmpakis G. and Froudakis G.E.

- 20th Panhellenic Chemistry Conference, Ioannina, Greece, September 20-23, 2005 (poster presentation)
  Mpourmpakis G. and Froudakis G.E.
- International Conference of Nanomaterials and Nanotechnologies (NN 2005), Crete, Greece, June 14-18, 2005 (poster presentation)
  Mpourmpakis G. and Froudakis G.E.
- 3rd International Conference "Computational Modeling and Simulation of Materials", Acireale (Catania), Sicily, Italy, 30 May - 4 June, 2004
- 19th Panhellenic Chemistry Conference, Heraklion, Greece, November 6-10, 2002 (poster presentation)
  Mpourmpakis G. and Froudakis G.E.
- XVIII Panhellenic Conference of Solid State Physics and Materials Science, 15-18 September 2002, Foundation for Research and Technology, Heraklion, Greece (poster presentation)
  Mpourmpakis G. and Froudakis G.E.
- Several talks in Panhellenic graduate student conferences and workshops (2001-2006)

TEACHING EXPERIENCE

Pitt teaching experience:

Spring 2015-2018: Instructor
Instructed the “CHE0200: Thermodynamics” course, one of the main pillar (6 credit) courses in the undergraduate curriculum of the Chemical Engineering Department at the University of Pittsburgh (number of students: ~70).
Overall Teaching Effectiveness Summary:
Year 2015: 4.18/5.00
Year 2016: 4.76/5.00
Year 2017: 4.51/5.00
Year 2018: 4.92/5.00

Fall 2016, 2017: Guest Lecturer
Designed and facilitated a workshop on preparing competitive applications for the National Science Foundation Graduate Research Fellowship Program (attendees ~30).

Fall 2017: Guest Lecturer
Guest-lectured by invitation the “Computational Catalysis: CO oxidation on Au” at the “Fundamentals of Reaction Processes” CHE2201 in the Chemical Engineering Department, University of Pittsburgh (attendees ~30).

Fall 2013: Workshop Instructor
Facilitated two training workshops (endnote, web of science, application package, interview process) on academic preparation of graduate students in the Chemical Engineering Department, University of Pittsburgh (attendees ~20).

Prior to Pitt teaching experience:

March, 2008, 2009, 2012: Guest Lecturer
Guest-Lectured by invitation the "Hydrogen Storage Problem" as part of the CHEG 614/867, "Special Topics in Energy Engineering" graduate course in the Chemical Engineering Department, University of Delaware (number of students 31).

January, 2010: Guest Lecturer
Facilitated training workshop on Quantum Mechanical Calculations using the Gaussian computational package for graduate students in the Chemical Engineering Department, University of Delaware (attendees ~20).

November, 2002 – June, 2004: Instructor
Designed and instructed the i) General Chemistry Laboratory (4 semesters) and ii) Physics Laboratory (2 semesters, 2003-2004) for undergraduates students in Technological Educational Institute of Crete, School of Health and Social Welfare, Department of Nutrition and Dietetics (number of students ~60).

September, 2002 – January, 2006: Teaching Assistant
Designed, supervised and graded (for instructor) projects in the graduate course "Computational Simulation Packages of Molecules", University of Crete, Chemistry Department (number of students ~10)

September, 2001 – January, 2003: Teaching Assistant
Designed and Led problem solving sessions and graded (for instructor) in the undergraduate courses of: i) Computational Chemistry (3 semesters), ii) Quantum Chemistry (2 semesters) and iii) Physics (1 semester) at the University of Crete, Chemistry Department (number of students in each course ~50)

ADVISING/SUPERVISING EXPERIENCE

Post-doctoral research advisees at Pitt:
Current:
- Mudit Dixit (January 2017 - present)

Graduate student advisees at Pitt:
PhD graduates:
- Pavlo Kostetskyy
  (2013-2018; PhD Thesis: Structure Activity Relationships in Acid-Catalyzed Alcohol Dehydration Reactions)
- Natalie Austin
  (2013-2018; PhD Thesis: Theoretical Investigation of CO_2 Activation and Chemical Conversion on Catalytic Nanoparticles, URM)

PhD in progress:
- Michael Taylor
  (2014-present; Expected graduation: May 2019; Passed Qualifiers; Project: Thermodynamic Stability of Metal Nanoparticles)

- James Dean
  (2016-present; Expected graduation: Aug. 2021; Passed Qualifiers; Project: Design of Optimal Bimetallic Nanoparticles)
- Michael Cowan
  (2017-present; Expected graduation: Aug. 2022; Passed Qualifiers, Project: Design of Ligand-Protected Bimetallic Nanoclusters)

MS graduates:
- Zihao Yan
  (2016-2018; May 2018; MS Thesis: Computational Modeling of Alloy Nanoparticle Stability)
- Xi Peng
  (2015-2017; MS thesis: First Principles Study of CO_2 Reduction on Mo_2C)

MS in progress:
- Robin Tan
  (2017-present; Expected graduation: May 2019; MS Thesis: Metal-Support Interactions)

Undergraduate student advisees at Pitt:

Mahmoud Ramadan (2018, REU from Ohio University, Project: Bimetallic Nanoparticle Stability)
Julia McKay (2018-present, Project: Thiolate Ligand Stability)
Eric Miller (2018-present, Project: Alkane Dehydrogenation)
Jonathan Estes (2017-present, Project: Hydration Reaction Equilibrium)
Mitchell Cholewinski (2017-2018, Project: Alkane Dehydrogenation)
Ashley Mascareno (2017, REU from ASU, Project: Bimetallic Nanoparticle Stability)
Macy Divens (2016, Project: Hydration Reaction Equilibrium)
John Hoover (2015, Project: Ligand-protected Nanoparticles)
Dania Faruqui (2015; visiting from NIT Maulana Azad India, Project: PM6 Method Performance)
Nick Zervoudis (2015-2016, Project: Alcohol Dehydration)
Isadora Carnaval (2015, Project: Pka Calculations of Acids)
Peter Tancini (2015-2017, Projects: i) Nanoparticles, ii) IR Spectra, iii) Microkinetic modeling)
Carly Nolan (2015, Project: Alkane Dehydrogenation)
Brandon Butina (2015, Project CO_2 Activation)
Jyoti Prakash Maheswari (2014, visiting from NIT Warangal India, Project: Alcohol Dehydration)
Olabobola Shobayo (2014, REU from UMBC, Project: Nanoparticle Growth, URM)
Tybur Casuse (2014, REU from UNM, Project: Adsorption on Metal Clusters, URM)

Prior to Pitt, at the University of Delaware:
Graduate students co-advised with Prof. Dionisios Vlachos: Vassili Vorotnikov, Nima Nikbin, Tim Courtney, Matthew Christiansen
Undergraduate student advisees: Stanley Herrmann, Shuting Feng

(URM=Underrepresented Minority Student)

SCHOLARSHIPS/AWARDS

August 2018:	Named "Emerging Investigator" by the ACS Journal of Chemical and Engineering Data
September 2017:	Named "Bicentennial Alumni Faculty Fellow" in Engineering (One of only 2 assistant professors throughout the School to receive an endowed faculty fellowship)
March 2017:	**National Science Foundation, CAREER Award**
December 2016:	James Pommersheim Award for Excellence in Teaching in Chemical Engineering
May 2016:	American Chemical Society (Petroleum Research Funds), Doctoral New Investigator
October 2015:	Elected from Pittsburgh Business Times "Who's Who in Energy"
August 2011:	Supporting Postdoctoral Researchers, Education and Lifelong Learning, Hellenic Republic-Ministry of Education and European Social Funds (E.U.)
June 2010:	Participated in the ***60th Nobel Laureates Meeting*** in Lindau-Germany, as a distinguished young researcher (An interdisciplinary meeting which brought together 500 young researchers who passed a multi-stage international selection procedure from around the globe, with Nobel Laureates from the fields of physiology, medicine, physics and chemistry).
May 2010:	Greek Army Deferment as "distinguished scientist"
January 2008:	People-Marie Curie Actions, International Outgoing Fellowships (FP7-PEOPLE-2007-4-1-IOF)
October 2005:	Stratis Sotirchos Award of "Best Research Work of New Scientist" in Panhellenic Symposium of Porous Materials. Demokritos, Athens, Greece
2002-2003:	I.K.Y. - Greek State Scholarship's Foundation (Master's Course Performance, rank 1st)
2001-2002:	University of Crete, Chemistry Department, Operational Programme for Education and Initial Vocational Training "Applied Molecular Spectroscopy" (Master's Course Performance, rank 1st)

NSF Graduate Research Fellowship Awards based on PI's Mentorship:

- Michael Taylor, joined the lab in December 2014, awarded the fellowship on May 2016: "Understanding Metal Nanoparticle Growth", 2016-2019, ***Funding: $225,060***
- Natalie Austin, joined the lab in December 2013, awarded the fellowship on May 2015: "CO_2 Hydrogenation to Methanol", 2015-2018, ***Funding: $225,060***

Pitt Student (advisees) other Awards:

- Natalie Austin received the Engineering Graduate Student Organization Award, as an outstanding Research Assistant in Chemical Engineering Department, at Pitt (2018)
- Natalie Austin received the Coull Award, as the best PhD student in the Department of Chemical Engineering, at Pitt (2017)
- James Dean received poster award in the Pittsburgh-Cleveland Catalysis Society Annual Meeting (2017)
- Natalie Austin has been selected to participate in the 67th Lindau Nobel Laureate Meeting (in Chemistry) after passing a multistage, worldwide selection process.
- Michael G. Taylor received poster award in the Advancing Research through Computing Conference (2017)

- Peter Tancini received the 1st place in "Computing and Process Control II" and the 1st prize in the "Computing and Simulation Technology Division" for his undergraduate poster presentation in AIChE 2016.
- Pavlo Kostetskyy received the AIChE Division of Catalysis and Reaction Engineering Student Travel Award (2016).
- Natalie Austin received the Women of Color STEM Conference Student Leadership Academic Award (2016).
- Peter Tancini receives the Pitt ΩXE Departmental Research Day 2nd undergraduate poster award (2016).
- Natalie Austin received the Pitt ΩXE Departmental Research Day 1st Graduate Poster Award (2016).
- Peter Tancini received the SSOE Undergraduate Summer Internship (2016).
- Peter Tancini received 3rd undergraduate poster award in AIChE 2015.
- Pavlo Kostetskyy received the Summer Term 2015 Outstanding PhD Paper Award
- Peter Tancini received a travel award for the AIChE 2015 undergraduate conference.
- Natalie Austin received the Fall Term 2014 Outstanding PhD Paper
- Natalie Austin received the first poster award in the Pittsburgh-Cleveland Catalysis Society Annual Meeting (2014).
- Natalie Austin was selected and sponsored to participate in the "Graduate Summer School: Electronic Structure Theory for Materials and (Bio)molecules", UCLA 2014.

RESEARCH FUNDING

Funded Grants at Pitt:

1) *Peer-Reviewed Federal Grants:*

"CAREER: Designing synthesizable, ligand-protected bimetallic nanoparticles and modernizing engineering curriculum through computational nanoscience", National Science Foundation (CBET), Program: Process Systems, Reaction Engineering and Molecular Thermodynamics, Period: 2017-2022, Role: PI.
Funding: $500,000

"Design of Optimal Bimetallic Nanoparticles", National Science Foundation (CMMI), Program: Design of Engineering Material Systems, Period: 2016-2019, Role: PI (Co-PIs: Prof. Götz Veser (Pitt), Prof. Chrysanthos Gounaris (CMU)).
Funding: $550,000 (Pitt: $350,395)

"Formation of Zeolites Responsible for Waste Glass Rate Acceleration: An Experimental and Computational Study for Understanding Thermodynamic and Kinetic Processes", Department of Energy, Program: Nuclear Energy University Program, Period: 2018-2021, Role: co-PI (PI: Prof. Jeffrey Rimer (U. Houston), co-PIs: Dr. James Neeway, Dr. Radha Motkuri and Dr. Jarrod Crum (Pacific Northwest National Laboratory).
Funding: $800,000 (Pitt: $280,012)

"Atomically Precise Au_{25}–based Alloy Nanoclusters for Electrochemical CO_2 Conversion", Department of Energy – National Energy Technology Laboratory, University Coalition for Fossil Energy Research (UCFER), Period: 2018-2020, Role: PI
Funding: $179,784

2) *Non-Peer-Reviewed Federal Grants*

"CO_2 Activation on Metal Carbides", U.S. Naval Research Lab., Period: 2016-2019, Role: PI.
Funding: $55,000 + $24,000 + $60,000 = $139,000

3) *Other Peer-Reviewed Funding Agencies:*

"Identifying Structure-Activity Relationships for the Dehydrogenation of Alkanes on Oxides", American Chemical Society, Petroleum Research Funds, Doctoral New Investigator Award, Period: 2016-2018, Role: PI, peer-reviewed.
Funding: $110,000

4) *Non-Peer-Reviewed Industrial Grants with Lubrizol:*

"Understanding PIB Functionalization Chemistries with first principles Calculations", Lubrizol Corporation, Period: 2017, Role: PI
Funding: $55,000

"Aminic Antioxidant Kinetic Modeling", Lubrizol Corporation, Period: 2015, Role: PI
Funding: $32,000

"Understanding Viscosity Creep using Quantum Mechanical Calculations", Lubrizol Corporation, Period: 2015, Role: PI
Funding: $40,000

"Separating isobutylene: in-silico screening of cation-exchanged zeolites", Lubrizol Corporation, Period: 2014, Role: PI
Funding: $25,000

5) *Peer-Reviewed Internal Pitt Grants:*

"Rational Design of Kidney Stone Growth Inhibitors from Quantum Mechanics", Central Research Development Funds, Office of Research and Research Council, University of Pittsburgh, Period: 2016-2018, Role: PI.
Funding: $14,000

"A Novel Process for Efficient, Decentralized Ammonia Synthesis", Mascaro Center for Sustainable Innovation, Period: 2016-2017, Role: Co-PI (PI: Prof. Götz Veser).
Funding: $47,132

"Nanocatalysis on thiolate-protected Au", Central Research Development Funds, Office of Research and Research Council, University of Pittsburgh, Period: 2014-2016, Role: PI.
Funding: $16,000

6) *Peer-Reviewed Grants for Access to National Computational Facilities:*

"Understanding "green" catalytic chemistries by first principles calculations", National Science Foundation, Extreme Science and Engineering Discovery Environment (XSEDE). Awarded access to supercomputing facilities, Role: PI, peer-reviewed.

Awarded resources value: $83,860 (corresponds to 987,514 comp. service units; Year: 2016)

Awarded resources value: $28,015 (corresponds to 843,160 comp. service units; Year: 2017)
Awarded resources value: $32,355 (corresponds to 974,683 comp. service units; Year: 2018)

Peer-reviewed Funded Grants prior to Pitt:
"Bimetallic Catalysts" Supporting Postdoctoral Researchers, Education and Lifelong Learning, Hellenic Republic-Ministry of Education and European Social Funds, E.U., Role: PI.
Funding: 150,000 euros (awarded and declined by PI)

"CO Oxidation on Au" People-Marie Curie Actions, International Outgoing Fellowships, European Commission, Period: 2008-2011, Role: PI.
Funding: 215,000 euros

"Hydrogen Storage in Nano-Materials for Fuel Cell Applications" PENED '03 (GR), Period: 2003-2006, Role: Researcher (PI: Prof. Froudakis.
Funding: 190,000 euros

"Novel energy storage materials: Theoretical investigation of hydrogen storage in carbon nanotubes and nanoscrolls" *PYTHAGORAS* '03 (GR), Period: 2003-2006 Role: Research Scholar (PI: Prof. Froudakis).
Funding: 80,000 euros

"Theoretical investigations of hydrogen storage in carbon nanotubes", Herakleitos '01 (GR), Period: 2001-2003, Role: Research Scholar (PI: Prof. Froudakis).
Funding: 33,000 euros

PARTICIPATION IN OTHER RESEARCH PROGRAMS (AS RESEARCHER)

2011-2013:	U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Award Number DE-SC0001004, CCEI-EFRC
2006-2008:	U.S. Department of Energy Award Number DE-FG02-05ER257022
2001-2004:	"EU-Growth AMMARE 2000"
2001:	"Ikyda 2001" Greek State Scholarship's Foundation – German Academic exchange service

ACADEMIC SERVICE AND LEADERSHIP

Departmental Service

- Coordinator of ChE Undergraduate Seminar Series for years 2014-2015, 2015-2016, 2016-2017, 2017-2018 (~350 students)
  - Organized more than 80 career development seminars for undergraduate students which included ~25 different companies (some presented multiple times).
- Recruiting Booth Faculty Participant in AICHE (2013, 2014, 2015, 2016 and 2017)
- PhD Qualifiers Committee member (2017)
- PhD and MS committee member for multiple students
- Pitt AIChE Student Chapter Mentor (2016)
  - Pitt Chem-E-Car placed 6th out of 28 at the 2016 AIChE Mid-Atlantic Conference
- Faculty Search Committee Member (2015)
  - Recruited female faculty (Fullerton)
- Graduate Admission Committee Member (2014)

- Undergraduate Program Committee (2017-present)
- Chemical Engineering Speaker for "So You Want to Become An Engineer" event (years: 2014, 2016)

Leadership
- President-Elect Pittsburgh-Cleveland Catalysis Society 2016-2018
- Organizer of Pittsburgh Cleveland Catalysis Society Annual Symposium (2018)
- Lead Organizer of all the Computational Catalysis Sessions at AIChE 2017
- Organizer (and Chair) of Computational Catalysis Symposium at ACS 2017 (Fall Meeting)
- Chair of Computational Catalysis session at AIChE2014, AIChE 2015, AIChE 2016, AIChE 2017 and AIChE 2018
- Chair of all poster sessions and member of organizing committee at NAM24 (North American Catalysis Society Meeting)
- Advisory Board of Center for Research Computing at the University of Pittsburgh

Reviewer for Funding Agencies
- National Science Foundation, USA
- Department of Energy, USA
- American Chemical Society, Petroleum Research Funds
- Engineering and Physical Sciences Research Council, United Kingdom
- The Research Foundation – Flanders (FWO), Belgium
- Central Research Development Funds (University of Pittsburgh)

Referee for 26 International Journals
- Nature Communications
- Journal of the American Chemical Society (JACS)
- Physical Review Letters
- ACS Catalysis
- Angewandte Chemie
- Journal of Catalysis
- Journal of Physical Chemistry (JPC)
- Physical Chemistry and Chemical Physics (PCCP)
- Journal of Chemical Physics (JCP)
- The European Physical Journal (EPJ)
- Catalysis Science and Technology
- Chemical Science
- Computational and Theoretical Chemistry (JCTC)
- Joule (RSC)
- Nanotechnology
- International Journal of Hydrogen Energy
- Applied Physics Letters (APL)
- Chemical Physics Letters (CPL)
- Journal of Physics: Condensed Matter
- Journal of Molecular Structure
- International Journal of Nanomedicine
- Journal of Molecular Catalysis A: Chemical
- Applied Catalysis A: General
- Computational Materials Science (COMMAT)
- Surface Science
- Industrial & Engineering Chemistry Research

General Scientific Community Service

- Invited and participated as panellist in a multi-university discussion on "How to prepare for faculty job applications" (2018)
- Invited and participated as panellist in the "How to build a research lab in the US as an international researcher" event of the Pitt-CMU postdoc association (2016).
- Evaluator for Graduate Programs for European Institutions.

Membership

American Chemical Society (ACS), American Institute of Chemical Engineers (AICHE), North America Catalysis Society (NACS)

ENHANCEMENT OF DIVERSITY

Awards of URM Student Advisees at Pitt

- Natalie Austin received the Engineering Graduate Student Organization Award, as an outstanding Research Assistant in Chemical Engineering Department, at Pitt (2018)
- Natalie Austin received the Coull Award, as the best PhD student in the Department of Chemical Engineering, at Pitt (2017)
- Natalie Austin has been selected to participate in the ***67th Lindau Nobel Laureate Meeting*** (in Chemistry) after passing a multistage, worldwide selection process (one of the only 4 Chemical Engineering students in the country to represent US).
- Natalie Austin received the ***Women of Color STEM Conference Student Leadership Academic Award*** (2016).
- Natalie Austin received the Pitt ΩXE Departmental Research Day 1st Graduate Poster Award (2016).
- Natalie Austin, received the ***NSF Graduate Research Fellowship*** (2015)
- Natalie Austin received the Fall Term 2014 Outstanding PhD Paper
- Natalie Austin received the first poster award in the Pittsburgh-Cleveland Catalysis Society Annual Meeting (2014).
- Natalie Austin was selected and sponsored to participate in the "Graduate Summer School: Electronic Structure Theory for Materials and (Bio)molecules", UCLA 2014.

URM Students Advised at Pitt

- Natalie Austin (PhD, National Science Foundation Fellow))
- Olabobola Shobayo (REU from UMBC)
- Tybur Casuse (REU from UNM)

Female Students Advised at Pitt

- Xi Peng (MS 2015-2017)
- Julia McKay (Undergraduate, 2018-present)
- Ashley Mascareno (Undergraduate 2017, REU from ASU)
- Macy Divens (Undergraduate 2016)
- Dania Faruqui (Undergraduate 2015; visiting from NIT Maulana Azad India)
- Isadora Carnaval (Undergraduate 2015)
- Carly Nolan (Undergraduate 2015)

Activities to Recruit URM and Female Students at Pitt

- Participated in undergraduate poster session in AIChE (2013, 2014, 2015, 2016 and 2017) and encouraged students to apply to Pitt.

- Participated in Pitt recruiting booth as faculty participant in AICHE (2013, 2014, 2015, 2016 and 2017) and presented ChE graduate program.
- Chemical Engineering Speaker for "So You Want to Become An Engineer" event (years: 2014, 2016)

Activities to Recruit URM and Female Faculty at Pitt

- Participates in the "Meet the Faculty" session of AIChE (2013, 2014, 2015, 2016), met and encouraged female and URM candidates to apply to Pitt
- Faculty Search Committee Member (2015)
    - Identified promising URM and female faculty candidates in AIChE
    - Interviewed candidates Laura Hirshfield, Dafne Klotsa, Susan Fullerton
    - Recruited female faculty (Fullerton)