

# ANDREAS HEYDEN

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Department of Chemical Engineering  
2C17 Swearingen Engineering Center  
University of South Carolina  
Columbia, SC 29208

Phone: +1 (803) 777-5025  
Fax: +1 (803) 777-8265  
Email: heyden@cec.sc.edu  
Web: www.cse.sc.edu/~heyden

## EDUCATION

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**Hamburg University of Technology** Hamburg, Germany

*Ph. D. in Chemical Engineering, December 2005*

Thesis: "Theoretical investigation of the nitrous oxide decomposition over iron zeolite catalysts"

Advisor: Professor Frerich J. Keil

Co-Advisor: Professor Alexis T. Bell Grade: "with distinction"

*Diplom in Chemical Engineering, December 2000 (undergraduate degree)*

Thesis: "Transition from molecular simulation of adsorption and diffusion to process simulation of a PSA module"

Advisor: Professor Günter Gruhn

Co-Advisor: Professor Frerich J. Keil Grade: "with distinction" (1.1)

*Vordiplom in Chemical Engineering, November 1997 (intermediate undergraduate degree)*

Grade: "very good" (1.1)

**University of California Berkeley** Berkeley, California

*Visiting scholar in the Department of Chemical Engineering, August – December 2001, August – December 2002, August 2003 – March 2004*

- Conducted research on Ph. D. thesis under Professor Alexis T. Bell. Attended various theoretical chemistry graduate classes.

*Graduate exchange student in Chemical Engineering, August 1998 – May 1999*

**University of Edinburgh** Edinburgh, UK

*Visiting scholar in the Department of Chemical Engineering, June – September 2000*

- Conducted research on Diploma thesis under Professor Nigel Seaton.

## PROFESSIONAL EXPERIENCE

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**University of South Carolina** Columbia Campus, South Carolina

**Department of Chemical Engineering**

*Professor*

*January 2018 – present*

*Graduate Director*

*January 2016 – present*

*Associate Professor*

*August 2014 – Dec. 2017*

*Assistant Professor*

*August 2007 – July 2014*

*Research areas: Computational (electro-)catalysis – Rational (nano)material design –*

*Multiscale modeling*

- Uncertainty quantification and machine learning in computational catalysis

- Study of the structure-performance relationship and rational design of systems relevant to (electro-) catalysis, energy production and storage, liquid hydrogen carriers, and plastics recycling.
- Study of the effect of catalyst support on the structure, surface composition, and catalytic activity of oxide supported metal ions, 2-dimensional materials, and metal clusters and nanoparticles.
- Heterogeneous catalysis at the solid-liquid interface for the conversion of lignocellulosic biomass model and platform molecules.
- Development of novel multi-scale modeling strategies and their application to hard and soft matter systems.

**Kyoto University**

Kyoto, Japan

**Fukui Institute of Fundamental Chemistry**

*Sabbatical in Prof. Morokuma's group*

*March 2015 – Aug. 2015*

*Research areas: Computational homogeneous catalysis – Machine Learning – Combustion*

**University of Minnesota**

Twin Cities Campus, Minnesota

**Department of Chemistry**

*Postdoctoral Fellow with Prof. Donald G. Truhlar*

*Nanomaterials subgroup*

*January 1, 2006 – August 1, 2007*

- Developed an adaptive partitioning method for combining multilevel methods such as QM/MM methods, with sampling schemes. Unlike previous QM/MM simulation algorithms, the method allows for the accurate study of processes in solution or the coupling of reaction to diffusion.
- Developed a conservative algorithm for an on-the-fly change of resolution in mixed atomistic / coarse-grained multiscale simulations.

**Hamburg University of Technology**

Hamburg, Germany

**Department of Chemical Engineering**

*Graduate Student Researcher with Prof. Frerich J. Keil and*

*Prof. Alexis T. Bell (UC Berkeley)*

*January 1, 2001 – December 31, 2005*

- Identified the active site and reaction mechanism of the N<sub>2</sub>O decomposition over iron zeolite catalysts – a catalytic system relevant for the reduction of greenhouse gas emissions from nitric and adipic acid plants.
- Gained significant insights into the nature of the catalytically active sites at different temperatures and the effects of species such as water and nitric oxide that have eluded experimentalists.
- Developed highly efficient algorithms for finding transition states on high-dimensional potential energy surfaces. Helped to integrate the methods into the new version of Q-Chem 3.0 and ChemShell and the next release of TURBOMOLE and VASP, four widely distributed quantum chemistry program packages.

*Undergraduate Student Researcher with Prof. Günter Gruhn*

*May – November 2000*

- Developed a configurational-biased Monte Carlo module for a Monte Carlo program and extended a molecular dynamics program to study molecules with internal constraints. Applied the programs to the study of adsorption and diffusion properties of small alkanes in multi-walled carbon nanotubes.
- Modeled the performance of a pressure swing adsorption module based on carbon nanotubes.

*Undergraduate Student Researcher with Prof. Frerich J. Keil*

*April – July 1998*

- Conducted experimental studies for the determination of a reaction rate equation for the methane combustion on a palladium catalyst.

**Bayer AG**

*External Consultant for Bayer Technology Services*

Leverkusen, Germany

*January 1 – December 31, 2001*

- Developed computer programs to predict the solubility of chemical compounds in pharmaceutically relevant solvents. Advised on multi-component solubility problems.

*Engineering Intern at Bayer Technology Services*

*August – November 1999*

- Developed programs to predict the affinity between macromolecules and solvent molecules to determine capsule material for aroma and drug substances. Conducted solubility experiments and improved a model for a stream dryer.

**Bran+Luebbe**

*Engineering Intern at Bran+Luebbe, Germany*

Norderstedt, Germany

*July 1 – September 30, 1994*

## AWARDS AND HONORS

- USC Educational Foundation Research Award for Science, Mathematics and Engineering, 2022
- USC College of Engineering and Computing Research Achievement Award, 2019
- USC Department of Chemical Engineering Publication Award, 2016
- USC College of Engineering and Computing Research Progress Award, 2016
- USC Department of Chemical Engineering Publication Award, 2014
- NSF CAREER Award, 2013 – 2019
- USC College of Engineering and Computing Young Investigator Research Award, 2013
- University of South Carolina Breakthrough Rising Star Award, 2012
- Minnesota Supercomputing Institute Research Scholarship; Postdoctoral Fellowship, Academic year 2006 – 2007
- Minnesota Supercomputing Institute Travel Grants; AIChE 2006 annual meeting and FOMMS 2006 meeting
- Council for the Lindau Nobel Laureate Meetings Participation Award; participant of the 18<sup>th</sup> Meeting of Nobel Prize Winners in Chemistry, Lindau, Germany; June 2006
- Karl H. Ditze Award; leading Ph.D. thesis at the Hamburg University of Technology, Academic year 2005 – 2006
- Ewald Wicke Foundation Travel Grant; AIChE 2005 annual meeting
- Bayer AG Mentoring Program Membership, April 2000 – May 2001
- German Academic Exchange Service Study Grant, Academic year 1998 – 1999
- Charitable Trust of the German Industry Study Grant, May 1997 – December 2000

CURRENT & PAST FUNDING (as PI: \$7,224,124; for AH as PI: \$5,566,290; for AH as co-PI/SI: \$3,558,292; Equipment Grant for USC as co-PI: \$498,525; \$\$\$ does not include Educational Grants)

Co-PI – “*Design of New Catalysts for the Generation of Clean H<sub>2</sub> from Liquid Organic Hydrogen Carriers: Dehydrogenation of Methylcyclohexane on Bimetallic Catalysts,*” \$3,181,725, 09/01/22 – 08/31/25, D. A. Chen (PI), A. Heyden (co-PI@\$600,000), J. Lauterbach (co-PI), J. Monnier (co-PI), K. Huang (co-PI), Department of Energy, Award No. DE-SC0023376.

PI – “*Collaborative Research: ECO-CBET: Coupled homogeneous and heterogeneous processes for an environmentally sustainable lignin-first biorefinery,*” \$860,000, 09/01/22 – 08/31/26, A. Heyden (PI@\$610,000), S. Ammal (co-PI), N. Berge (co-PI), National Science Foundation, Award No. 2218938.

Co-PI – “*EFRI E3P: Hydrogenolysis for upcycling of polyesters and mixed plastics,*” \$2,000,000, 09/01/21 – 08/31/25, J. W. Medlin (PI), A. Heyden (co-PI@\$440,000), National Science Foundation, Award No. EFMA-2132033.

SI – “*REU Site: CO2 Chemical Engineering: Opportunities and Challenges,*” \$413,036, 08/01/21 – 08/31/24, C. Williams (PI), Lauterbach (co-PI), A. Heyden (SI@\$0), National Science Foundation, Award No. EEC-2050956.

PI – “*Development of Computational Models for Polymer Scission,*” \$2,500, 05/01/21 – 10/31/22, A. Heyden, M. Burns (undergraduate student), Magellan of USC.

PI – “*Development of Computational Models for Polymer Scission,*” \$2,000, 05/10/21 – 08/13/21, A. Heyden, M. Burns (undergraduate student), McNAIR Junior Fellows (MJF) of USC.

Co-PI – “*Institute for Cooperative Upcycling of Plastics (iCOUP),*” \$12,800,000, 10/01/20 – 9/30/24, A. Sadow (PI), A. Heyden (co-PI@\$600,000), US Department of Energy, Office of Basic Energy Sciences, Award No. DE-AC-0207CH11358.

PI – “*Theoretical Investigation of Heterogeneous Catalysis at the Solid-Liquid Interface for the Conversion of Lignocellulosic Biomass Model Molecules,*” \$550,000, 09/01/20 – 08/31/23, US Department of Energy, Office of Basic Energy Sciences, Award No. SC0007167.

PI – “*Methane Partial Oxidation over Multifunctional 2-D Materials,*” \$1,261,624 (\$1,000,000 federal, \$261,624 cost share), 03/20/20 – 03/15/23, A. Heyden (PI@\$400,000 federal, \$110,456), W. Medlin (co-PI@\$400,000 federal, \$100,000 cost share), Pajarito Powder (co-PI@\$200,000 federal, \$51,168 cost share), US Department of Energy, NETL, Award No. DE-FE0031878.

PI – “*Statement of Work for Institute for Cooperative Catalysis in Upcycling of Polymers (iCOUP),*” \$55,000, 09/01/19 – 12/31/20, US Department of Energy, Office of Basic Energy Sciences, Subcontract from Ames Lab.

Co-PI – “*CC\* Networking Infrastructure: Building a Science DMZ for Data-intensive Research and Computation at the University of South Carolina,*” \$498,525, 10/01/19 – 09/30/21, J. Crichigno (PI), A. Heyden (co-PI), National Science Foundation, Award No. OAC-1925484.

PI – “*Statement of Work for Institute for Cooperative Catalysis in Upcycling of Polymers (iCOUP),*” \$55,000, 09/01/18 – 08/31/19, US Department of Energy, Office of Basic Energy Sciences, Subcontract from Ames Lab.

Co-PI – “*Understanding and Designing Novel Anode Materials for Solid Oxide Fuel Cells,*” \$640,000, 06/01/18 – 05/31/21, F. Chen (PI), A. Heyden (co-PI@\$320,000), S. Ammal (co-PI), National Science Foundation, Award No. DMR-1832809.

PI – “*Collaborative Research: Understanding and Manipulating the Solvent Microenvironment for Selective, Catalytic Amination of Renewable Oxygenates,*” \$225,000, 06/01/18 – 05/31/21, National Science Foundation, Award No. CBET-1805307.

PI – “*Theoretical Investigation of Heterogeneous Catalysis at the Solid-Liquid Interface for the Conversion of Lignocellulosic Biomass Model Molecules,*” \$500,000, 09/01/17 – 08/31/20, US Department of Energy, Office of Basic Energy Sciences, Award No. SC0007167.

PI – “*International Collaboration for Understanding Catalyst Deactivation and Designing Durable Catalysts*,” \$50,000, 1/01/17 – 12/31/17, A. Heyden (PI), USC VPR and ECHE Department.

PI – “*Accelerating Computational Analysis of Hydrocarbon Combustion Reactions using Machine Learning Techniques*,” \$3,000, 10/01/16 – 6/30/17, A. Heyden, E. Grace (undergraduate student), Science Undergraduate Research Fellowship Program of USC.

Co-PI (USC site leader) – “*RII Track-2 FEC: Center for a Sustainable Water, Energy, and Food Nexus (SusWEF)*,” \$4,000,000, (USC share: \$1,797,000), 08/01/16 – 07/31/20, N. Cardona-Martinez (PI), J. Lopez-Garriga (co-PI), A. Heyden (co-PI@837,841), M. Curet-Arana (co-PI), G. Terejanu (co-PI), National Science Foundation, Award No. OIA-1632824.

PI – “*Collaborative Research: SusChEM: Rational Design of Non-Precious Metal Catalysts for a Future Biorefining Industry*,” \$300,000, 06/01/16 – 05/31/20, National Science Foundation, Award No. CHEM-1565964.

PI – “*Explore Innovative Chemistry of Natural Gas Conversion to DME*,” \$210,000, 3/15/16 – 09/30/17, A. Heyden (PI@\$97,000), D. A. Chen, F. Chen, DOE SRNL subcontract.

PI – “*DMREF: Collaborative Research: Design and Discovery of Multimetallic Heterogeneous Catalysts for a Future Biorefining Industry*,” \$840,000, 09/01/15 – 08/31/19, A. Heyden (PI@\$570,000), S. C. Ammal, G. Terejanu (co-PI@\$270,000), National Science Foundation, Award No. CBET-1534260.

PI – “*Reductive Deoxygenation of Glycerol over a Pt(111) Surface*,” \$3,000, 05/01/15 – 10/31/15, A. Heyden, A. Yonge (undergraduate student), Magellan of USC.

PI – “*Theoretical Investigation of Heterogeneous Catalysis at the Solid-Liquid Interface for the Conversion of Lignocellulosic Biomass Model Molecules*,” \$380,000, 09/01/14 – 08/31/17, US Department of Energy, Office of Basic Energy Sciences, Award No. SC0007167.

SI – “*Collaborative Research: Planning Grant: I/UCRC for the Center for Rational Catalyst Synthesis*,” \$15,850, 04/01/14 – 03/31/15, J.R. Regalbuto, A. Heyden (SI@\$0), National Science Foundation, Award No. IIP-1361943.

SI – “*REU Site: Cradle to the Grave – CO<sub>2</sub> Opportunities and Challenges*,” \$343,143, 04/01/14 – 03/31/17, J. Lauterbach, A. Heyden (SI@\$0), National Science Foundation, Award No. EEC-1358931.

Co-PI – “*Design and Discovery of Novel Electrode Materials for Reversible Solid Oxide Cells*,” \$100,000, 05/01/13 – 07/31/14, F. Chen (PI@\$40,000), A. Heyden (co-PI@\$35,000), H. zur Loye (co-PI@\$25,000), ASPIRE-II Program of USC.

PI – “*CAREER: Uncertainty Quantification in the Rational Design of Bifunctional Catalysts*,” \$400,000, 07/01/13 – 06/30/18, National Science Foundation, Award No. CBET-1254352.

PI – “*Collaborative Research: Rational Design of Bifunctional Catalysts for the Conversion of Levulinic Acid to  $\gamma$ -valerolactone*,” \$250,000, 09/01/12 – 08/31/15, National Science Foundation, Award No. CBET-1159863.

PI – “*Rational Design of Selective Hydrodeoxygenation Catalysts for Organic Acids*,” \$400,000, 08/16/12 – 07/31/14, A. Heyden (PI@\$200,000), C. T. Williams (co-PI@\$100,000), J. Monnier (co-PI@\$100,000), National Science Foundation, Award No. CHEM-1153012.

PI – “*Catalytic Conversion of Biomass-Derived Platform Molecules into High Octane Biofuels*,” \$100,000, 05/01/12 – 07/31/13, A. Heyden (PI@\$33,334), C. T. Williams (co-PI@\$33,333), R. D. Adams (co-PI@\$33,333), ASPIRE-II Program of USC.

PI – “*Theoretical Investigation of Heterogeneous Catalysis at the Solid-Liquid Interface for the Conversion of Lignocellulosic Biomass Model Molecules,*” \$450,000, 09/01/11 – 08/31/14, US Department of Energy, Office of Basic Energy Sciences, Award No. SC0007167.

Co-PI – “*Fuel Flexible Advanced Power for Portable Applications,*” \$3,600,000, 10/01/10 – 09/30/11, G. Hilton (PI), A. J. Lauterbach (co-PI), K. Reifsnider (co-PI), B. Benicewicz (co-PI), A. Heyden (co-PI@\$76,845), Defense Advanced Research Projects Agency, Contract No. W91CRB-10-1-0007.

PI – “*Computational Investigation of Aqueous-Phase Processing for Hydrogen Production,*” \$20,000, 04/01/10 – 06/30/11, Resource Opportunity Program of USC.

Co-PI – “*Catalytic Liquid-Phase Deoxygenation of Biomass to Hydrocarbon Fuels for Transportation and Stationary Applications,*” \$150,000, 09/01/09 – 08/31/10, C. T. Williams (PI), F. Chen (co-PI), A. Heyden (co-PI@\$50,000), USC NanoCenter and Future Fuels Program.

Co-PI – “*Development of Ultra-low Loading Platinum Alloy Cathode Catalysts for PEM Fuel Cells: Theoretical and Experimental Studies,*” \$300,000, 03/15/10 – 03/14/13, B. Popov (PI), P. Ganesan (co-PI), A. Heyden (co-PI@\$16,915), National Science Foundation, Award No. CBET-0966956.

PI – “*Multiscale Modeling of Bifunctional Catalysts for the Water-Gas-Shift Reaction,*” \$300,000, 08/01/09 – 05/31/12, National Science Foundation, Award No. CBET-0932991.

Co-PI – “*Energy Frontier Research Center (EFRC) for Science Based Nano-Structure and Synthesis of Heterogeneous Functional Materials for Energy Systems,*” \$17,691,001, 09/01/09 – 07/31/14, K. Reifsnider (PI) A. Heyden (co-PI@\$581,691), US Department of Energy, Office of Basic Energy Sciences, Award No. DE-SC0001061.

## TEACHING EXPERIENCE

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### University of South Carolina

Columbia, South Carolina

#### Research group members

##### Research Associate Professors

- Salai Cheettu Ammal (5/2022 – present) – “Multiscale Modeling of Bifunctional (Electro-) Catalysts”

##### Postdoctoral Associates

- Jong Hyuk Park (12/2007 – 11/2008) – “Development of Multiscale Modeling Methods for Complex Soft Matter Systems” – currently at UNIST – Ulsan National Institute of Science and Technology, Republic of Korea
- Salai Cheettu Ammal (3/2008 – 9/2013) – “Multiscale Modeling of Bifunctional (Electro-) Catalysts”
- Jianmin Lu (12/2009 – 11/2014) – “Catalytic Hydrodeoxygenation of Biomass to Green Diesel” and “Fuel Flexible Advanced Power for Portable Applications” – currently at Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China
- Vijay Solomon Rajadurai (3/2014 – 2/2016) – “Catalytic Hydrodeoxygenation of Biomass Model Molecules” – currently Assistant Professor at Madras Christian College, India
- Yongjie Xi (11/2016 – 7/2020) – “Catalytic Hydrodeoxygenation of Biomass Model Molecules”
- Supriya Saha (1/2017 – 8/2017) – “Oxidative and Reductive Propane Dehydrogenation” – currently at CSIR-NEIST, Jorhat, India

- Biplab Rajbanshi (1/2018 – 8/2020) – “Oxidative and Reductive Propane Dehydrogenation”, Assistant Professor, Department of Chemistry, Visva-Bharati University, Santiniketan, West Bengal, India
- Anand Verma\*\* (1/2018 – 6/2018) – “Catalytic Hydrodeoxygenation of Biomass Model Molecules” \*\*official status visiting intern.
- Wenqiang Yang (5/2020 – 6/2021) – “Rational Design of Multimetallic Catalysts for the Hydrodeoxygenation of Succinic Acid”
- Mohammad Saleheen (9/2020 – 2/2022) – “Condensed Phase Modeling in Heterogeneous Catalysis”
- Subrata Kundu (10/2022 – present) – “Condensed Phase Reaction Modeling in Porous Systems”

#### *Graduate Students*

- Suwit Suthirakun (Fall 2008 – May 11, 2013) – Ph.D. thesis title: “Rational Design of Perovskite Based Anode Materials for Solid Oxide Fuel Cells: A Computational Approach”  
Currently Assistant Professor at Suranaree University of Technology, Thailand
- Sara Aranifard (Spring 2009 – May 11, 2013) – Ph.D. thesis title: “Theoretical Investigation of the Water-Gas Shift Reaction at the Three-Phase Boundary of Ceria Supported Platinum Metal Clusters”  
Sept. 2011 - winning third place at the poster competition at the 10<sup>th</sup> Annual Symposium of the Southeastern Catalysis Society in Asheville, NC  
2011 Kokes Award for the 22<sup>nd</sup> North American Catalysis Society Meeting  
Currently Instructure at Azad University, Iran
- Mian Muhammad Faheem (Fall 2009 – August 15, 2014) – Ph.D. thesis title: “Theoretical Investigation of Aqueous-Phase Processing of Oxygenated Hydrocarbons”  
2014 – Winner of the USC Chemical Engineering Outstanding Graduate Student Award  
Currently Associate Professor at the University of Engineering & Technology Lahore, Pakistan
- Sina Behtash (Spring 2010 – December 15, 2014) – Ph.D. thesis title: “Theoretical Investigation of the Catalytic, Liquid-Phase Hydrodeoxygenation of Organic Acids and Esters”  
2015 – Winner of the USC Chemical Engineering Graduate Student Research Award  
Currently working at Sealed Air Corp.
- Eric Walker\* (Fall 2013 – August 15, 2016) – Ph.D. thesis title: “Uncertainty Quantification in the Rational Design of Catalytic Surfaces”  
USC Presidential fellowship; 2014 Eastman Fellowship; 2015 AIChE CRE Division Travel Grant  
Sept. 2014 – winning third place at the oral presentation competition at the 13<sup>th</sup> Annual Symposium of the Southeastern Catalysis Society in Asheville, NC  
Currently Computational Scientist & Research Assistant Professor at SUNY Buffalo.
- Md. Osman Mamun (Fall 2012 – August 15, 2017) – Ph.D. thesis title: “Rational Design of Bifunctional Catalysts for the Conversion of Levulinic Acid to  $\gamma$ -Valerolactone”  
Sept. 2013 – winning second place at the poster competition at the 12<sup>th</sup> Annual Symposium of the Southeastern Catalysis Society in Asheville, NC  
2017 Kokes Award Winner for the 25<sup>th</sup> North American Catalysis Society Meeting  
Currently at New Equilibrium Bio
- Mohammad Saleheen (Fall 2013 – August 15, 2019) – Ph.D. thesis title: Theoretical Investigation of Liquid-Phase Processing of Biomass Model Molecules

- 2016 Eastman fellowship award; 2018 AIChE CRE Division Travel Grant  
 2019 – Winner of the USC Chemical Engineering Graduate Student Research Award
- Asif Jamil Chowdhury\*\* (Fall 2015 – May 15, 2020) – Ph.D. thesis title: A Machine Learning Based Approach to Accelerate Catalyst Design
  - Wenqiang Yang (Fall 2015 – May 15, 2020) – Ph.D. thesis title: Rational Design of Multimetallic Catalysts for the Hydrodeoxygenation of Succinic Acid
- 2019 Kokes Award for the 26<sup>th</sup> North American Catalysis Society meeting
- Charles Fricke (Fall 2016 – May 15, 2022) – Ph.D. thesis title: Rational Design of Propane Dehydrogenation Catalysts
  - Kyung-eun You (Fall 2016 – December 15, 2021) – Ph.D. thesis title: First-Principles Based Heterogeneous Catalyst Design for Energy Conversion and Plastics Upcycling Processes
- 2020 AIChE WIC Travel Award winner
- Subrata Kundu (Spring 2017 – September 30, 2022) – Ph.D. thesis title: Theoretical Investigation of Liquid-Phase Processing of Biomass Model Molecules on metals and zeolites
  - Mehdi Zare (Fall 2017 – August 15, 2021) – Ph.D. thesis title: Solvent Effect Modeling in Heterogeneous Catalysis
- 2021 – Winner of the USC Chemical Engineering Graduate Student Research Award
- Dia Sahseh (Fall 2018 – present) – Ph.D. thesis title: Understanding and Manipulating the Solvent Microenvironment for Selective, Catalytic Amination of Renewable Oxygenates
  - Nicholas Szaro (Fall 2018 – present) – Ph.D. thesis title: Understanding and Designing Anode Materials for Solid Oxide Fuel Cells Operating on Methane
  - Olajide Bamidele (Fall 2019 – present) – Ph.D. thesis title: Plastics upcycling by hydrogenolysis
  - Panuwat Watthaisong (Spring 2021 – present) – Ph.D. thesis title: Rational catalyst design for a lignin-first biorefinery
  - Mubarak Bello (Spring 2021 – present) – Ph.D. thesis title: Plastics upcycling by  $\beta$ -alkyl elimination chemistry
  - Emmanuel Eluno (Spring 2022 – present) – Ph.D. thesis title: Hydrogenolysis for upcycling of polyesters and mixed plastics
  - Paratee Komen (Spring 2022 – present) – Ph.D. thesis title: Theoretical Investigation of Liquid-Phase Processing of Biomass Model Molecules
  - Bhawana Rayamajhi (Summer 2022 – present) – Ph.D. thesis title: Theoretical Investigation of the Dehydrogenation of Liquid Organic Hydrogen Carriers

\*Co-advised with Prof. Gabriel Terejanu

\*\*Computer Science Student: Co-advised with Prof. Gabriel Terejanu

#### *Undergraduate Students*

- George Hearn - USC (5/2008 – 5/2009)
- Gregory McCumber – Youngstown State University (5/2010 – 7/2010)
- Stephanie Haag – Montana State University (5/2011 – 7/2011)
- Ryan McLay – Florida Institute of Technology (5/2012 – 7/2012)
- Donald Mitchell – City University of New York (5/2014 – 7/2014)
- Nick Eigenbrot – USC (5/2014 – 8/2015)
- Adam Yonge – USC (12/2014 – 8/2017)
- Madeline Ley – Oklahoma State University (5/2016 – 7/2016)
- Utid Suriya – Chiang Mai University (5/2016 – 7/2016)
- Elizabeth Grace – USC (9/2016 – 2/2018)
- Celine Tesvara – Penn State University (6/2018 – 7/2018)



- Marie Burns – USC (8/2020 – present)

*Classes taught as Professor*

- ECHE 730: Chemical reactor design; Fall 2007, Fall 2008, Spring 2016
- ECHE 722: Advanced Mass Transfer; Spring 2009, Spring 2010, Spring 2011, Spring 2012, Spring 2013, Spring 2017, Spring 2018, Spring 2020, Spring 2022
- ECHE 589H, 789H: Multiscale Modeling: From Electrons to Chemical Reactors (developed elective course); Spring 2009
- ECHE 589, 789: Heterogeneous Catalysis: A Perspective from a Computational Scientist; Spring 2014, Spring 2019, Spring 2021, Spring 2023
- ECHE 430: Chemical Engineering Kinetics; Fall 2010, Fall 2011, Fall 2012, Fall 2013, Fall 2014, Fall 2015, Fall 2016, Fall 2017, Fall 2018, Fall 2019, Fall 2020, Fall 2021, Fall 2022

**Hamburg University of Technology**

Hamburg, Germany

*Graduate Student Instructor*

- Supervised one Master's thesis, two diploma theses, and five undergraduate research projects, 2001 – 2004
- Supervised four lab courses in chemical reaction engineering, Spring 2001 – 2004
- Presented tutorials in linear algebra, Academic year 2001 – 2002
- Supervised students in two process design courses, Spring 2001 and 2002

**Refugee House**

Hamburg, Germany

*Volunteer Instructor*

- Taught African refugees calculus, German, and MS Office, 2001 – 2003

**ADDITIONAL EXPERIENCE**

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**Student Parliament, Hamburg University of Technology**

Hamburg, Germany

*Finance committee member*

May 1996 – April 1998

- Approved and revised budget proposals. Informed students about the European credit transfer system.

**German Army**

Heide, Germany

*Compulsory military service in the Army Medical Corps*

October 1994 – September 1995

**PROFESSIONAL MEMBERSHIPS**

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Electrochemical Society. Member 2012 – present

American Chemical Society. Member 2006 – present

Computational Molecular Science and Engineering Forum. Member 2005 – present

American Institute of Chemical Engineers. Member 2003 – present

Alumni Society of the Charitable Trust of the German Industry. Member 2001 – present

**PROFESSIONAL ACTIVITIES**

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2023 NAM29 organizing committee, Scientific Chair, conference will take place in June 2025 in Atlanta

2022 NAM29 organizing committee, Scientific Chair, conference will take place in June 2025 in Atlanta

2022 NSF Panel Review

2022 Ad-Hoc Grant Review, DOE BES

2022 Interviewing PhD scholarship applicants for the sdw (Stiftung der Deutschen Wirtschaft)

2021 NSF Panel Review

2021 Interviewing PhD scholarship applicants for the sdw (Stiftung der Deutschen Wirtschaft)

2021 DOE BES PNNL Catalysis Program Review

2021 Ad-Hoc Grant Review, DOE BES

2021 ACS Spring 2021 Meeting Symposium Co-Organizer and Co-Chair

2020 Ad-Hoc Grant Review, DOE BES

2020 NSF Panel Review

2020 ICC Co-chair of session “Theory and Computation in Catalysis” - cancelled

2019 NAM Co-chair of session “Modeling and Simulation of Catalysis: Machine Learning Applications”

2019 NSF Panel Review

2019 Ad-Hoc Grant Review, DOE BES

2018 Ad-Hoc Grant Review, DOE EERE

2018 Ad-Hoc Grant Review, DOE BES

2018 Ad-Hoc Grant Review, NSF

2018 ACS Spring 2018 Meeting Symposium Co-Organizer and Co-Chair

2017 Session Chair at NAM meeting

2017 DOE BES Program Proposal Review

2017 2 x NSF Panel Review

2016 Ad-Hoc Grant Review, DOE BES

2016 3 x NSF Panel Review

2015 Top 2% reviewer for ACS Catalysis

2015 NSF Panel Review

2015 Ad-Hoc Grant Review, NSF

2014 Top 1% reviewer for ACS Catalysis

2014 Ad-Hoc Grant Review, DOE BES

2014 Ad-Hoc Grant Review, European Research Council (ERC)

2014 Ad-Hoc Grant Review, ACS Petroleum Research Fund

2014 NSF Panel Review

2013 NSF Panel Review

2013 Invited reviewer for “Large Scale Production Computing and Storage Requirements for Basic Energy Sciences: Target 2017” organized by the DOE BES, ASCR, and NERSC

2013 Participant at the Materials Genome Initiative (MGI) Grand Challenges Workshop organized by DOE-BES and NSF

2013 Ad-Hoc Grant Review, NSF

2013 Ad-Hoc Grant Review, DOE ASCR ALCC program

2013 Session Chair at the 23<sup>rd</sup> NAM

2012 Ad-Hoc Grant Review, Department of Energy (BES)

2011 NSF Panel Review

2011 Ad-Hoc Grant Review, ACS Petroleum Research Fund

2010 Co-Organizer of 2010 Southeast Theoretical Chemistry Association (SETCA) Annual Meeting at the University of South Carolina, SC

2010 NSF Panel Review

- 2009-2013 Initiated a mentoring program and lecture series on “Next Energy” at the Engineering Academy of Columbia High School
- 2008-Present Session Chair and co-Chair, Annual Meeting of the American Institute of Chemical Engineers
- 2008 NSF Panel Review
- 2008-Present Member of the ChemShell (versatile hybrid QM/MM program package) developer’s team
- 2008 Ad-Hoc Grant Review, DTRA Basic Research Program
- 2007-Present Manuscript Review for ACS Catalysis; ACS Sustainable Chemistry & Engineering; AIChE Journal; Angewandte Chemie, Applied Catalysis A; Applied Catalysis B; Applied Physics Letters; Carbohydrate Research; Catalysis Communications; Catalysis Science & Technology; Catalysis Letters; Chemical Engineering Science; Chemical Physics Letters; Chemistry of Materials; Computer Physics Communications; Energy & Fuels; Environmental Science & Technology; Green Chemistry, Industrial & Engineering Chemistry Research; International Journal of Hydrogen Energy; International Journal of Quantum Chemistry; Journal of Alloys and Compounds; Journal of Catalysis; Journal of Chemical Physics; Journal of Chemical Theory and Computation; Journal of Cluster Science; Journal of Computational Chemistry; Journal of Materials Chemistry; Journal of Molecular Catalysis A; Journal of Physical Chemistry; Journal of Physical Chemistry Letters; Journal of Power Sources; Journal of Solid State Chemistry; Journal of the American Chemical Society; Molecular Simulation; Nature Publishing Group, Physical Chemistry Chemical Physics; RSC Catalysis Series; Science Advances; Soft Materials; Surface Science
- 2000-Present Developed highly efficient algorithms for finding transition states on high-dimensional potential energy surfaces, molecular dynamics codes for mixed resolution systems, Monte Carlo codes to study adsorption, and methods for calculating rates of reactions occurring at solid-liquid interfaces. Transition state search algorithms are available upon request and are used in industry (e.g., Evonic Degussa GmbH) and academia. Programs developed have also been implemented into Q-Chem, ChemShell, TURBOMOLE, and VASP, four widely distributed electronic structure program packages.

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