John A. Keith

Contact Information

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Research Interests

Computational chemistry for catalysis and sustainability - specific applications reaction mechanism studies for solar fuels, electrochemical reactions, anticorrosion coatings, and green chemical design.

Education

California Institute of Technology, Pasadena, CA USA

Ph.D., Chemistry, September 2007

- Dissertation: "Computational Insight into Homogeneous Organopalladium Catalysis"
- Advisor: William A. Goddard, III

Wesleyan University, Middletown, CT USA

B.A., Chemistry with High Honors, May, 2001

- Advisor: George A. Petersson

Academic Experience

University of Pittsburgh (Pitt), Pittsburgh, Pennsylvania USA
Department of Chemical and Petroleum Engineering (CHE)

- R. K. Mellon Faculty Fellow in Energy — Sep. 2013 – present
- Associate professor — Sep. 2019 – present
- Assistant professor — Sep. 2013 – Aug. 2019

Princeton University, Princeton, New Jersey USA
Department of Mechanical and Aerospace Engineering

- Associate Research Scholar — Nov. 2010 – Jul. 2013
- Advisor: Emily A. Carter
- Instructor — Feb. 2013 – May. 2013
  APC509: Methods and Concepts in Electronic Structure Theory

Universität Ulm, Ulm, GERMANY
Institut für Elektrochemie

- Alexander von Humboldt Postdoctoral Fellow — Oct. 2007 – Oct. 2010
- Advisor: Timo Jacob

Honors and Awards

- Luxembourg National Research Fund: INTER Mobility award — 2019
- R.K. Mellon Faculty Fellowship — 2013 – present
- NSF-CAREER Award — 2017
- Journal of Materials Chemistry A - Emerging Investigator Issue — 2017
- Pittsburgh Business Times: Who's Who in Energy — 2014 – 2016
- Alexander von Humboldt Postdoctoral Fellowship — 2008 – 2010
- Phi Beta Kappa — 2001
- American Chemical Society: Connecticut Valley Regional Award — 2001
- Bradley Prize for Outstanding Undergraduate Thesis in Chemistry — 2001
- American Chemical Society Analytical Chemistry Award — 2000

Media

- **Pittsburgh WESA:** Highlighted in Weekly Pittsburgh Tech Report (27 June 2017) http://bit.ly/2ubVaEj
- **Pittsburgh WESA:** Reseacher Finds Possible Way to Make CO_2 Into Energy (3 Feb. 2015) http://bit.ly/1WfC9aU
- **Pittsburgh Business Times:** Pitt researcher receives funding to study carbon dioxide recycling (24 Jul. 2015) http://bit.ly/1TTY48W
- **Quoted in Science Magazine:** There's too much carbon dioxide in the air. Why not turn it back into fuel? (10 Sep. 2015) http://bit.ly/1K1xrZQ

Service

Pitt / Departmental Service

- Bridging program coordinator — Sep. 2019 – present
- Graduate student recruiting coordinator — Sep. 2013 – Aug. 2017

Pitt / Swanson School of Engineering (SSoE)

- SSoE Diversity Committee Representative for CHE — Sep. 2016 – present
- SSoE Committee for updating graduate applications — June 2016

National Service

- Physical Chemistry (PHYS) Division Officer for ACS, energy subdivision (three-year term) — Jan. 2016 – Dec. 2018
- Symposium co-organizer 2017 Fall ACS meeting, PHYS division: "Spectroscopic and Computational Insights into Solid/Liquid Interfaces for Energy Conversion" (with Dr. Katherine Jungjohann) — Aug. 2017
- Symposium co-organizer 2017 Spring ACS meeting, COMP division: "State-of-the-Art Methods for Modeling Materials Chemistry" (with Prof. Benjamin Janesko) — Apr. 2017
- Conference co-organizer and session coordinator, Midwest Theoretical Chemistry Conference, Pittsburgh, PA (with Profs. Ken Jordan, Daniel Lambrecht, Jeffry Madura) — Jun. 2016
- Co-chair for AIChE 2015 annual meeting, Catalysis and Reaction Engineering Division: "Computational Catalysis", Salt Lake City, UT — Nov. 2015
- Co-chair for AIChE 2015 annual meeting, Computational Molecular Science and Engineering Forum: "Recent Advances in Molecular Simulation Methods", Salt Lake City, UT. — Nov. 2015
- Website/publicity co-chair and session organizer 24th North American Catalysis Society Meeting, Pittsburgh, PA. — Jun. 2015
- Intel ISEF 2015 - Grand Award Judge — May 2015

• Symposium co-organizer 2015 Spring ACS meeting, CATL division: "Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis" (with Prof. Amanda Morris) — Mar. 2015

• Co-chair for AIChE 2014 annual meeting, Catalysis and Reaction Engineering Division: "Computational Catalysis V", Atlanta, GA. — Nov. 2014

• Co-chair for AIChE 2014 annual meeting, Computational Molecular Science and Engineering Forum: "Recent Advances in Molecular Simulation Methods 1 & 2", Atlanta, GA. — Nov. 2014

• Co-chair for AIChE 2013 annual meeting, Catalysis and Reaction Engineering Division: "Applications of DFT+X in Catalysis II" San Francisco, CA. — Nov. 2013

Scientific Reviewing

AAAS:	Sci. Rep.
ACS:	ACS Books; ACS Catal.; Chem. Rev.; Environ. Sci. Technol.; Ind. Eng. Chem. Res.; Inorg. Chem.; J. Am. Chem. Soc.; J. Chem. Theory Comput.; J. Org. Chem.; J. Phys. Chem. C; J. Phys. Chem. Lett; Organometallics
AIP:	J. Chem. Phys.
APS:	Phys. Rev. Lett.
ECS:	J. Electrochem. Soc.
Elsevier:	Acta Mater.; Catal. Today; Chem. Eng. Sci.; Chem. Phys.; Coord. Chem. Rev.; Electrochim. Acta; Electrochem. Commun; J. Catal.; J. Power Sources, Mater. Chem. Phys.; Surf. Sci.
IOP:	J. Phys. Condens. Matter
NPG:	Nature Commun.; Nature Mater.; Nature Chem.; Nature Energy
RSC:	Catal. Sci. Technol.; Dalton Trans.; Energy Environ. Sci.; J. Mater. Chem. A; Nanoscale; Phys. Chem. Chem. Phys.
Springer:	Electrocatal.; J. Solid State Electrochem.; Theor. Chem.Acc.
Wiley:	Angew. Chem. Int. Ed.; Chem. Eur. J.; Eur. J. Org. Chem.
Grant proposals:	Reviewer for NSF; DOE; AFOSR; American Chemical Society Petroleum Research Fund; Kentucky Science & Technology Corporation; NWO (Netherlands Organisation for Scientific Research); DFG (German National Science Foundation)

Teaching

University of Pittsburgh

• CHE 0400 (5 credit) — Summer 2019
Reactive Process Engineering
Undergraduate pillar course in chemical engineering kinetics

• CHE 0400 (5 credit) — Spring 2019
Reactive Process Engineering
Undergraduate pillar course in chemical engineering kinetics

• CHE 0400 (5 credit) Summer 2018
Reactive Process Engineering
Undergraduate pillar course in chemical engineering kinetics

• CHE 2101 (3 credit) Spring 2018
Fundamentals of Thermodynamics
Graduate-level chemical engineering thermodynamics & statistical mechanics

• CHE 0400 (5 credit) Summer 2017
Reactive Process Engineering
Undergraduate pillar course in chemical engineering kinetics

• CHE 1017/2017 (3 credit) Spring 2016
Chemical Energy & Nature of the Chemical Bond
Elective course in applications of quantum mechanics in chemistry

• CHE 2101 (3 credit) Fall 2015
Fundamentals of Thermodynamics
Graduate-level chemical engineering thermodynamics & statistical mechanics

• CHE 1017/2017 (3 credit) Spring 2015
Chemical Energy & Nature of the Chemical Bond
Elective course in applications of quantum mechanics in chemistry

• CHE 2101 (3 credit) Fall 2014
Fundamentals of Thermodynamics
Graduate-level chemical engineering thermodynamics

• Center for Simulation and Modeling Workshop May 7 – 9, 2014
Three lectures in quantum chemistry

Princeton University – overall teaching effectiveness scores given (5.0 is highest score)

• APC509 (3 credit) Spring 2013
Methods and Concepts in Electronic Structure Theory
Graduate level course in applications of quantum mechanics in chemistry

Funding

Total external funding to date: $1,473,789

• NSF (CHE-1856460) Jan. 2020 – Dec. 2023
Collaborative Research: Regulating homogeneous and heterogeneous mechanisms in six-electron water oxidation
Role: PI, Amount awarded: **$222,789**, PI time: 0.5 month

• Luxembourg National Research Fund Aug. 2019 – Jun. 2020
INTER-Mobility: Enhancing Atomistic Modeling: Physically Robust Atomistic Machine Learning Models for Predictive Insights into Solvated Chemical Reactions
Amount awarded: **$89,000**, in support of 10-month visit

• Naval Research Laboratory (N00173191G006) Apr. 2019 – Sep. 2019
Quantum chemistry studies of cathodic reactions on Cr_2O_3 surfaces
Role: PI, Amount awarded: **$49,994**, PI time: 2 months

• Naval Research Laboratory (N00173181G002) Nov. 2017 – May 2018
First principles QM predictions of dopants that suppress corrosion on Ti-6Al-4V oxides
Role: PI, Amount awarded: **$49,850**, PI time: 2 months

• NSF (CBET-1705592) Aug. 2017 – Jul. 2020
SusChEM: Machine learning blueprints for greener chelants
Role: PI (with co-PI Eric Beckman), Amount awarded: **$299,999**, PI time: 0.5 month

• NSF (CBET-1653392) Feb. 2017 – Jan. 2022
CAREER: SusChEM: Unlocking local solvation environments for energetically efficient hydrogenations with quantum chemistry
Role: PI, Amount awarded: **$526,746**, PI time: 1.0 month

• Naval Research Laboratory (N00173161G023) Aug. 2016 – Jan. 2017
Quantifying the effect of solvation on anti-corrosion coatings
Role: PI, Amount awarded: **$50,000**, PI time: 0.5 month

• Naval Research Laboratory (N00173151G018) Oct. 2015 – Apr. 2016
Preventing Corrosion by Controlling Cathodic Reaction Kinetics
Role: PI, Amount awarded: **$75,000**, PI time: 1 month

• ACS Petroleum Research Fund Jul. 2015 – Jun. 2017
Unraveling Heterocycle-Promoted Hydride Transfer Mechanisms for Energetically Efficient Fuel and Petrochemical Production
Role: PI, Amount awarded **$110,000**, PI time: 0.4 month

Internal funding: $\sim$ $66,000

• Mascaro Center for Sustainable Innovation (Pitt) Jul. 2017 – Jun. 2018
Seed grant: Toward machine learning blueprints for greener chelants
Role: PI, Amount awarded: **$50,000**, PI time: 0 months

• Pitt Central Research Development Fund (CRDF) Jul. 2015 – Jun. 2017
Towards a Robust and Efficient Computational Modeling Approach for Elucidating Fundamental Photocatalysis
Role: PI, Amount awarded **$16,000**, PI time: 0 months

Students at Pitt

Postdocs

• Aude Marjolin Jan. 2014 – Oct. 2014
Former program manager for Pittsburgh Quantum Institute

• Victor Oyeyemi Jul. 2014 – Jun. 2015
Currently data scientist for Bloomberg

Ph. D. students

- Mitchell C. Groenenboom (Pitt CHE) — Jan. 2014 – Apr. 2018
  R.K. Mellon Graduate Fellow (2013-2018), National Research Council-funded postdoc at NIST, and now data scientist for Brembo

- Karthikeyan Saravanan (Pitt CHE) — Jan. 2014 – Dec. 2018
  Pittsburgh Quantum Institute Graduate Fellow (2016) and currently data scientist at Highmark in Pittsburgh

- Yasemin Basdogan (Pitt CHE) — Jan. 2016 – Jan. 2020
  currently postdoc at Caltech

- Charles Griego (Pitt CHE) — Jan. 2018 – present
  R.K. Mellon Graduate Fellow (2018-2019), NSF graduate research fellow (2019-2022)

- Alex Maldonado (Pitt CHE) — Jan. 2018 – present
  NSF graduate research fellow honorable mention (2019)

- Lingyan Zhao (Pitt CHE) — Jan. 2020 – present

- Barbaro Zulueta (Pitt CHE) — May 2020 – present

Thesis MS students

- Yaqun Zhu (Pitt CHE) — Jan. 2014 – Jul. 2015

- Nguyen Vo (Pitt CHE, co-advised with Karl Johnson) — Jan. 2015 – Apr. 2017

Special project MS students

- Junchao Mei (Pitt CHE) — Sep. 2017 – Dec. 2017

- Benjamin Carlson (Pitt CHE) — Jan. 2017 – Apr. 2017

Undergraduate students (working more than 6 months)

- Eli Lipsman (Pitt CHE) — Jun. 2020 – present
  2020 SSoE summer undergraduate

- Brian Gentry (Pitt MEMS) — Jun. 2018 – present
  2019 SSoE summer undergraduate

- Sarah Newton (Pitt CHE) — Jan. 2017 – Aug. 2017
  2018 MCSI summer undergraduate

- Ethan Henderson (Pitt CHE) — Jan. 2017 – Apr. 2019
  2017 MCSI summer undergraduate

• Angela Leo (Pitt CHE) 2017 MCSI summer undergraduate 2018 SSoE summer undergraduate	Jan. 2017 – Apr. 2019
• Charles Hansen (Pitt CHE)	Sep. 2016 – Apr. 2017
• Yinan Kang (Pitt CHE)	Sep. 2014 – Sep. 2015
• Jeffrey Carr (Pitt CHE)	Jan. 2014 – Apr. 2015
• Rohith Amruthur (Pitt CHE)	Jan. 2014 – Dec. 2014

Visiting students

• Peter Fatouros (summer REU student from Clarkson University)	Jun. 2019 – Aug. 2019
• William Belfield (visiting student from University of Loughborough)	Feb. 2018 – Jun. 2018
• Caelin Celani (summer REU student from Washington and Jefferson University)	Jun. 2017 – Aug. 2017
• James Dean (summer REU student)	Jun. 2015 – Jul. 2015
• Dinesh Sundaravadivelu Devarajan (undergraduate visitor) Currently graduate student at Texas Technological University	Jun. 2015 – Jul. 2015
• Eric Gottlieb (visiting Carnegie Mellon University chemistry PhD student)	Jan. 2014 – Jun. 2015
• Alyssa Shorak (high school student)	Jun. 2015 – Sep. 2015
• Gina Wagner (summer REU student from Trine University)	Jun. 2014 – Jul. 2014

PRESENTATIONS

Invited Presentations since arriving at Pitt, '' denotes pending talk, '‡' denotes virtual seminar given due to COVID-19*

46.‡	EPFL Lausanne, Switzerland **Title:** Local Solvation In Chemistry and Some Alchemy	May. 5, 2020
45.‡	Christian-Albrechts-Universität zu Kiel Kiel, Germany **Title:** Local Solvation In Chemistry and Some Alchemy	Apr. 30, 2020
44.‡	Danish Technical University Copenhagen, Denmark **Title:** Local Solvation In Chemistry and Some Alchemy	Apr. 29, 2020
43.‡	MPI-Hamburg Hamburg, Germany **Title:** Local Solvation In Chemistry and Some Alchemy	Apr. 28, 2020

42.‡ KU Leuven — Apr. 27, 2020
Leuven, Belgium
Title: Local Solvation In Chemistry and Some Alchemy

41.‡ University of Basel — Apr. 1, 2020
Basel, Switzerland
Title: Local Solvation In Chemistry and Some Alchemy

40. University of Ulm (Germany) — Feb. 20, 2020
Ulm, Germany
Title: Local Solvation In Chemistry: What's Important, and How to Model It Effectively

39. 2019 Telluride Workshop on Computational Materials Chemistry — Jul. 17, 2019
Telluride, CO
Title: Economical explorations of physical reaction mechanisms

38. Yale University — Jun. 27, 2019
New Haven, CT
Title: Computational quantum chemistry modeling of local solvation

37. Wesleyan University — Jun. 26, 2019
Middletown, CT
Title: Mostly computational quantum chemistry modeling of local solvation?and a little bit of alchemy

36. Center for Energy Seminar Series — Jan. 14, 2019
University of Pittsburgh, Pittsburgh, PA
Title: How quantum chemistry can save humanity

35. Chemical Physics Seminar — Oct. 5, 2018
Caltech, Pasadena, CA
Title: Computational alchemy and paramedic treatments for continuum solvation modeling

34. Seminar: Department of Chemistry — Sep. 6, 2018
Trinity University, San Antonio, TX
Title: Computational elucidation of local solvation effects in chemistry

33. Workshop: "CECAM: Machine Learning at Interfaces" — Jun. 6, 2018
EPFL, Lausanne, Switzerland
Title: Opportunities for modeling complex systems with machine learning

32. CATL division session "Machine Learning for Catalysis Research" — Mar. 19, 2018
255th ACS meeting, New Orleans, LA
Title: Applications of machine learning for studying amorphous materials

31. CATL division session "Unconventional Catalysis - Targeting Stable Molecules" — Mar. 19, 2018
255th ACS meeting, New Orleans, LA
Title: Computational searches for energetically efficient CO_2 reduction reaction steps across chemical and materials space

30. CATL division session "Activation of light (C1-C4) hydrocarbons. Theory and experiments" — Mar. 22, 2018
255th ACS meeting, New Orleans, LA
Title: Screening hydrocarbon activation pathways with computational alchemy

29. Seminar: Department of Chemistry — Feb. 16, 2018
University of Virginia, Charlottesville, VA
Title: In silico searches for (in)efficient electrocatalysts through chemical and material compound space

28. Mesilla Workshop on Nanocatalysis — Feb. 5, 2018
Mesilla, NM
Title: Computational searches for energetically (in)efficient electrocatalysts

27. Seminar: Department of Chemical and Biomolecular Engineering — Jan. 18, 2018
University of Illinois, Urbana, IL
Title: In silico searches for (in)efficient electrocatalysts through chemical and material compound space

26. Computational Chemistry/Computational Modeling Meeting — Sep. 12, 2017
U.S. Army Corps of Engineers, Vicksburg, MS
Title: In silico searches for energetically (in)efficient electrocatalysts through chemical and material compound space
presented by Mitchell C. Groenenboom

25. ENFL division session "Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application" — Aug. 22, 2017
254th ACS meeting, Washington, DC
Title: Pourbaix diagrams to guide searches for CO_2 reduction catalysts

24. Philadelphia Conference in Theoretical Chemistry (PCTC) — Aug. 18, 2017
University of Pennsylvania, Philadelphia, PA
Title: In silico searches for energetically (in)efficient electrocatalysts through chemical and material compound space

23. Seminar: National Energy Technology Laboratory, Pittsburgh, PA — Apr. 12, 2017
Title: In silico searches for energetically (in)efficient catalysts through chemical and material compound space

22. Seminar: Department of Materials Science and Engineering — Feb. 3, 2017
Carnegie Mellon University, Pittsburgh, PA
Title: In silico searches for energetically (in)efficient catalysts through chemical and material compound space

21. Seminar: Department of Chemistry and the Center for Photochemical Sciences — Jan. 18, 2017
Bowling Green State University, Bowling Green, OH
Title: In silico searches for renewable energy catalysts through chemical and material compound space

20. Seminar: Department of Chemical and Biomolecular Engineering — Nov. 11, 2016
Drexel University, Philadelphia, PA
Title: In silico searches for renewable energy catalysts through chemical and material compound space

19. Seminar: Theory Department — Oct. 11, 2016
Army Research Laboratory, Aberdeen, MD
Title: In silico searches for renewable energy catalysts through chemical and material compound space

18. Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA — Sep. 23, 2016
Title: In silico searches for renewable energy catalysts through chemical and material compound space

17. CATL division session "Electrocatalysis for CO_2 reduction" — Aug. 24, 2016
252th ACS meeting, Philadelphia, PA
Title: Tailoring materials for electrocatalytic reduction of CO_2
presented by Karthikeyan Saravanan

16. Workshop: Exploring Chemical Space with Machine Learning and Quantum Mechanics — Jun. 1, 2016
CECAM workshop, ETH Zurich, Switzerland
Title: How to search for alloy catalysts using computational alchemy

15. ENFL division session "Application of Computational Chemistry for Fuel and Energy Production" — Mar. 16, 2016
251th ACS National Meeting, San Diego, CA
Title: First-principles investigations of aqueous phase CO_2 reduction by borohydrides

14. CATL division session "Condensed Phase Catalysis Symposium" — Mar. 15, 2016
251th ACS National Meeting, San Diego, CA
Title: Mapping the energetically efficient catalysis of renewables with Pourbaix diagrams

13. I^2CNER International Workshop "CO_2 capture and utilization division", — Feb. 4, 2016
Kyushu University, Fukuoka, Japan
Title: Atomic scale design of molecules and materials for energetically efficient electrochemical CO_2 reduction

12. I^2CNER Annual Symposium "Computational solutions to fundamental problems in carbon-neutral energy research" — Feb. 1, 2016
Kyushu University, Fukuoka, Japan
Title: Current status of and outlook for experimental and computational synergies to study electrocatalytic energy conversion

11. 2016 Electrochemistry Gordon Research Conference — Jan. 11, 2016
Ventura, California
Title: Computational determination of molecular co-catalysts for energetically efficient electrochemical processes

10. COMP division session "Calculating pKas and Redox Potentials" — Aug. 18, 2015
250th ACS National Meeting, Boston, MA
Title: Redox Potential and pKa Descriptors for Exploring the Catalysis of Renewables

9. Seminar at LONI Institute/LA-SiGMA — Apr. 1, 2015
Louisiana State University, Baton Rouge, LA
Title: Exploring CO_2 conversion into commodity chemicals with first principles quantum chemistry

8. Session: "The Science of CO_2 Capture in Energy Production" — Oct. 31, 2014
ACS Central Regional Meeting 2014, Pittsburgh, PA
Title: Unraveling mechanistic aspects of heterocycle-promoted CO_2 electroreduction with quantum chemistry

7. Pitt Center for Simulation and Modeling symposium: "Advancing Research Through High Performance Computing" — Oct. 15, 2014
University of Pittsburgh, PA
Title: Engineering CO_2 recycling with high-performance computing

6. ENFL division session "Applications of Theoretical Chemistry for Energy and Fuel Production" — Aug. 12, 2014
248th ACS National Meeting, San Francisco, CA
Title: First principles descriptors for identifying molecular co-catalysts that facilitate efficient electroreductions for renewable energy

5. PHYS division session "Renewable Energy Generation at the Interface between Theory and Experiment" — Aug. 11, 2014
248th ACS National Meeting, San Francisco, CA
Title: Unraveling mechanistic aspects of heterocycle-promoted CO_2 electroreduction with quantum chemistry

4. Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA — Jun. 02, 2014
Title: Unraveling heterocycle-promoted CO_2 electroreduction with quantum chemistry
presented by Aude Marjolin

3. ENFL division session "Innovations in Carbon Dioxide Capture, Storage, Conversion, and Utilization" — Mar. 16, 2014
247th ACS National Meeting, Dallas, TX
Title: Unraveling heterocycle-promoted CO_2 electroreduction with quantum chemistry

2. Seminar at Joint Center for Artificial Photosynthesis (JCAP) — Oct. 18, 2013
Caltech, Pasadena, CA
Title: Quantum mechanical insights into photoelectrochemical CO_2 reduction processes

1. PHYS division symposium: "Physical Chemistry of Solar Energy Conversion" — Sep. 08, 2013
246th ACS National Meeting, Indianapolis, IN
Title: Quantum mechanical insights into photoelectrochemical CO_2 reduction processes

Contributed presentations since arriving at Pitt, '**S**' *- denotes student presentations*

40. 2017 AIChE Annual Meeting, Minneapolis, MN — Nov. 2, 2017
S **Title:** Accelerated Catalyst Screening Using Computational Alchemy
Oral presentation by Karthikeyan Saravanan

39. 2017 AIChE Annual Meeting, Minneapolis, MN — Oct. 30, 2017
S **Title:** Elucidating and Correcting the Unreliability of Continuum Solvation Methods When Modeling Homogeneous Reaction Mechanisms
Oral presentation by Yasemin Basdogan

38. 2017 AIChE Annual Meeting, Minneapolis, MN — Oct. 30, 2017
S **Title:** The Mechanism of Isobutylene Polymerization: New Insight into Proton-Catalyzed Polymerizations
Oral presentation by Minh Nguyen Vo

37. 232nd ECS Meeting, National Harbor, MD — Oct 5, 2017
Title: Galvanic Corrosion of AA7075-T6 Caused By Doped Titanium Oxides in a Controlled Atmospheric Environment
Oral presentation by Dr. Steven Policastro

36. 232nd ECS Meeting, National Harbor, MD — Oct 4, 2017
S **Title:** Understanding Electrochemical Reduction of CO_2 Using Quantum Chemistry Modeling
Oral presentation by Karthikeyan Saravanan

35. 254th ACS meeting, Washington, DC — Aug 23, 2017
S **Title:** Deoptimizing oxygen reduction reaction catalysis with doped amorphous Ti oxides
Oral presentation by Mitchell C. Groenenboom

34. 254th ACS meeting, Washington, DC — Aug 22, 2017
S **Title:** Elucidating and correcting the unreliability of continuum solvation methods when modeling homogeneous reaction mechanisms
Oral presentation by Yasemin Basdogan

33. 25th North American Catalysis Society Meeting, Denver, CO — Jun 5, 2017
S **Title:** The mechanism of isobutylene polymerization: new insight into proton-catalyzed polymerizations from the growing string method
Oral presentation by Minh Nguyen Vo

32. Pittsburgh Cleveland Catalysis Society, Akron, OH — May 25, 2017
S **Title:** Accurate computational modeling of chemical reactions in polar solvents using cluster-continuum modeling
Oral presentation by Yasemin Basdogan

31. 253rd ACS meeting, San Francisco, CA — Apr. 6, 2017
Title: Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 coatings for corrosion inhibition
Oral presentation

30. 16th Annual AIChE, San Francisco, CA — Nov. 18, 2016
S **Title:** Alloy Catalyst Discovery Using Computational Alchemy
Oral presentation by Karthikeyan Saravanan

29. 16th Annual AIChE, San Francisco, CA — Nov. 16, 2016
S **Title:** First Principles Quantum Chemistry Calculations to Model CO_2 Electroreduction on SnO_2 Particles
Oral presentation by Karthikeyan Saravanan

28. 16th Annual AIChE, San Francisco, CA — Nov. 15, 2016
S **Title:** Neural Network and Reaxff Comparison for Au Properties
Oral presentation by Jacob Boes, CMU student

27. 16th Annual AIChE, San Francisco, CA — Nov. 15, 2016
S **Title:** Comparing the Effect of Counter Ions, Solvent Molecules, and Electron Correlation on Homogeneous Reaction Models
Oral presentation by Mitchell C. Groenenboom

26. Electrochemical Energy Symposium, CMU, Pittsburgh, PA — Oct. 21, 2016
S **Title:** Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 surfaces
Oral presentation by Mitchell C. Groenenboom

25. 252th ACS meeting, Philadelphia, PA — Aug. 24, 2016
S **Title:** Tailoring materials for electrocatalytic reduction of CO_2
Oral presentation by Karthikeyan Saravanan

24. 252th ACS meeting, Philadelphia, PA — Aug. 22, 2016
S **Title:** Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 surfaces
Oral presentation by Mitchell C. Groenenboom

23. PQI2016, Pittsburgh, PA — Apr. 20, 2016
S **Title:** Traversing the chemical space - Alloy catalysts discovery using Alchemy
Oral presentation by Karthikeyan Saravanan

22. PQI2016, Pittsburgh, PA — Apr. 20, 2016
S **Title:** Explicitly unraveling the roles of counter ions and solvent molecules
Poster presented by Mitchell C. Groenenboom

21. 15th Annual AIChE, Salt Lake City, UT — Nov. 11, 2015
Title: Liquid Mixtures Freezing at Room Temperature: More Insights into Crystallization and Applications of Poly(trimethylene glycol)/Water Mixtures
Oral presentation

20. 15th Annual AIChE, Salt Lake City, UT — Nov. 9, 2015
Title: New Perspectives on Aqueous Phase Reaction Mechanisms with Ab Initio Molecular dynamics, Nudged-Elastic Band, and Wavefunction Theory-in-DFT Embedding
Oral presentation

19. 15th Annual AIChE, Salt Lake City, UT — Nov. 8, 2015
Title: Coincidences and Insights into Molecular Heterocycles That Catalyze CO_2 Reduction with Low Overpotentials
Oral presentation

18. 228th Electrochemical Society meeting, Phoenix, AZ — Oct 11, 2015
S **Title:** Exploring the non innocence of inorganic complex ligands in (photo)electrochemical CO_2 reduction
Oral presentation by Karthikeyan Saravanan

17. Science2015 hosted by the Pittsburgh Quantum Institute, Pittsburgh, PA — Oct. 8, 2015
S **Title:** Aqueous phase CO_2 reduction with sodium borohydride: An ab initio molecular dynamics and nudged-elastic band mechanistic study
Poster presentation by Mitchell C. Groenenboom

16. Catalysis in Energy Group Poster Fair, Pittsburgh, PA — Aug. 11, 2015
S **Title:** Aqueous phase CO_2 reduction with sodium borohydride: An ab initio molecular dynamics and nudged-elastic band mechanistic study
Poster presentation by Mitchell C. Groenenboom

15. 24th North American Catalysis Society Meeting, Pittsburgh, PA — Jun. 19, 2015
S **Title:** Nitrogen Enriched Nanocarbons as a Metal-Free Water Reducing Catalysts
Oral presentation by Eric Gottlieb

14. 24th North American Catalysis Society Meeting, Pittsburgh, PA — Jun. 17, 2015
S **Title:** The Mechanism for C-H Borylation By Cu-Fe Heterobimetallic Catalysts (Poster)
Poster presented by Yaqun Zhu

13. 24th North American Catalysis Society Meeting, Pittsburgh, PA — Jun. 16, 2015
S **Title:** Pourbaix Diagrams of Ruthenium Chromophores Under CO_2 Reduction Conditions
Oral presentation by Karthikeyan Saravanan

12. 24th North American Catalysis Society Meeting, Pittsburgh, PA — Jun. 16, 2015
S **Title:** Unraveling the Electrochemical Reactivities of Aromatic N-Heterocycles with Quantum Chemistry
Oral presentation by Mitchell C. Groenenboom

11. 249th ACS National Meeting, Denver, CO — Mar. 25, 2015
Title: First-principles quantum chemical investigations on the selectivity of borohydride for carbon dioxide and bicarbonate reduction in protic conditions
Oral presentation

10. 249th ACS National Meeting, Denver, CO — Mar. 24, 2015
S **Title:** Aqueous phase CO_2 reduction with sodium borohydride: An ab initio molecular dynamics and nudged-elastic band mechanistic study (Poster)
Oral presentation by Mitchell C. Groenenboom

9. 14th Annual AIChE, Atlanta, GA — Nov. 19, 2014
Title: Water-Induced Crystallization of Poly(trimethyleneglycol)
Oral presentation by Prof. Robert Enick

8. 14th Annual AIChE, Atlanta, GA — Nov. 18, 2014
Title: Thermochemical Descriptors for Unraveling Molecular Promoted CO_2 Conversions
Oral presentation

7. 14th Annual AIChE, Atlanta, GA — Nov. 17, 2014
S **Title:** First Principles Quantum Chemical Modeling of Radium in Barite for Fracking Wastewater Remediation
Poster presented by Gina Wagner

6. 14th Annual AIChE, Atlanta, GA — Nov. 17, 2014
Title: Benchmarking Modern Range Separated DFT Functionals and Ab Initio Wavefunction Theory-in-DFT Embedding for Computational Catalysis Applications
Oral presentation

5. Catalysis in Energy Group meeting, Pittsburgh, PA — Nov. 5, 2014
S **Title:** A combined AIMD/NEB mechanistic study of aqueous phase CO_2 reduction with sodium borohydride
Oral presentation by Mitchell C. Groenenboom

4. 2014 ACS Central Regional Meeting, Pittsburgh, PA — Oct. 30, 2014
Title: Unraveling mechanistic aspects of heterocycle-promoted CO_2 electroreduction with quantum chemistry
Oral presentation

3. 2014 ACS Central Regional Meeting, Pittsburgh, PA — Oct. 30, 2014
S **Title:** Investigations of nitrogen doping density in graphene and hydrogen adsorption by DFT
Oral presentation by Eric Gottlieb

2. 2014 ACS Central Regional Meeting, Pittsburgh, PA Oct. 29, 2014
S **Title:** Preventing corrosion by controlling cathodic reaction kinetics
Poster presented by Victor B. Oyeyemi

1. 2014 ACS Central Regional Meeting, Pittsburgh, PA Oct. 29, 2014
S **Title:** Aqueous phase CO_2 reduction with sodium borohydride: An ab initio molecular dynamics and nudged-elastic band mechanistic study.
Poster presented by Mitchell C. Groenenboom

Peer reviewed journal publications (work at Pitt without prior mentors)

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