John A. Keith

Contact Information

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Research Interests

Computational chemistry for catalysis and sustainability. Specific applications in 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

- R. K. Mellon Faculty Fellow in Energy — Sep. 2013 – present
- Tenure-track Assistant Professor in CHE — Sep. 2013 – present

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

- 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
- insidehighered.com: Mover and Shaker — 2013
- 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

Patents

- Peilin Liao, John A. Keith, Emily A. Carter. Reducing Overpotentials in Hematite Photoanode Photoelectrochemical Cells by Doping. Princeton Docket No. 12-2755-1. **Filed 11/1/2012**

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 / Swanson School of Engineering (SSoE)

• Pitt STRIVE/SSoE Diversity Committee Representative for CHE	Sep. 2016 – present
• Pitt CHE Graduate student recruiting coordinator. *Contributed to increasing Ph.D. student enrollment of underrepresented minority students. Recognized by Associate Dean of Diversity Affairs, Dr. Sylvanus Wosu*	Sep. 2013 – Aug. 2017
• Pitt SSoE Committee for updating graduate applications	June 2016
• Coordinator for Pitt Classroom Connection (outreach program with the Pittsburgh Science and Technology Academy)	Jan. 2015 – Jun. 2015

National Service

• Physical Chemistry (PHYS) Division Officer for ACS, Energy Subdivision	Mar. 2016 – present
• Symposium organizer 2017 Fall ACS meeting, PHYS division: "Spectroscopic and Computational Insights into Solid/Liquid Interfaces for Energy Conversion"	Aug. 2017
• Symposium organizer 2017 Spring ACS meeting, COMP division: "State-of-the-Art Methods for Modeling Materials Chemistry"	Apr. 2017
• Conference co-organizer and session coordinator, Midwest Theoretical Chemistry Conference, Pittsburgh, PA	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 organizer 2015 Spring ACS meeting, CATL division: "Theoretical and Experimental Synergies at the Frontiers of Renewable Energy Catalysis"	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 I & 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.
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:	DOE ad hoc reviewer; NSF panelist; NSF ad hoc reviewer; ACS-PRF; Kentucky Science & Technology Corporation; NWO (Netherlands Organisation for Scientific Research)

Teaching

University of Pittsburgh – Office of Measurement and Evaluation of Teaching (OMET) overall teaching effectiveness scores given (5.0 is highest score).

• CHE 0400 (5 credit)	Summer 2017
Reactive Process Engineering	OMET: 4.23/5.0
Undergraduate pillar course in chemical engineering kinetics	enrollment: 18
• CHE 1017/2017 (3 credit)	Spring 2016
Chemical Energy & Nature of the Chemical Bond	OMET: 4.00/5.0
Elective course in applications of quantum mechanics in chemistry	enrollment: 6

• CHE 2101 (3 credit) — Fall 2015
Fundamentals of Thermodynamics — OMET: 3.44/5.0
Graduate-level chemical engineering thermodynamics & statistical mechanics — enrollment: 30

• CHE 1017/2017 (3 credit) — Spring 2015
Chemical Energy & Nature of the Chemical Bond — OMET: 4.27/5.0
Elective course in applications of quantum mechanics in chemistry — enrollment: 16

• CHE 2101 (3 credit) — Fall 2014
Fundamentals of Thermodynamics — OMET: 3.50/5.0
Graduate-level chemical engineering thermodynamics — enrollment: 22

• 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 — 4.1/5.0
Graduate level course in applications of quantum mechanics in chemistry — enrollment: 12

Funding

External funding: ∼ $1,035,000

• 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: **$500,000**, 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: ∼ $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

• Yasemin Basdogan (Pitt CHE) — Jan. 2016 – present

• Mitchell C. Groenenboom (Pitt CHE) — Jan. 2014 – present
Expected graduation spring 2018

• Karthikeyan Saravanan (Pitt CHE) — Jan. 2014 – present
Expected graduation winter 2018

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

Thesis MS students

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

Special project MS students

• Junchao Mei (Pitt CHE) — Sep. 2017 – present

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

Undergraduate students (working more than 6 months)

• Ethan Henderson (Pitt CHE) — Jan. 2017 – present

• Angela Leo (Pitt CHE) — Jan. 2017 – present

• 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

- Caelin Celani (summer REU student) — Jun. 2017 – Aug. 2017
- James Dean (summer REU student) — Jun. 2015 – Jul. 2015
- Dinesh Sundaravadivelu Devarajan (undergraduate visitor) — Jun. 2015 – Jul. 2015
  Currently graduate student at Texas Technological University
- Eric Gottlieb (visiting CMU chemistry PhD student) — Jan. 2014 – Jun. 2015
- Alyssa Shorak (high school student) — Jun. 2015 – Sep. 2015
- Gina Wagner (summer REU student) — Jun. 2014 – Jul. 2014

PRESENTATIONS

Invited Presentations since arriving at Pitt, '' denotes pending talk*

31.	255th ACS meeting; CATL division session "Machine Learning for Catalysis Research", New Orleans, LA	*Mar. 2018
30.	255th ACS meeting; CATL division session "Unconventional Catalysis - Targeting Stable Molecules", New Orleans, LA	*Mar. 2018
29.	255th ACS meeting; CATL division session "Activation of light (C1-C4) hydrocarbons. Theory and experiments", New Orleans, LA	*Mar. 2018
28.	Department of Chemistry, University of Virginia, Charlottesville, VA	*Feb. 16, 2018
27.	Mesilla Workshop on Nanocatalysis, Mesilla, NM	*Feb. 2018
27.	Department of Chemical and Biomolecular Engineering, University of Illinois, Urbana, IL	*Jan. 18, 2018
26.	Computational Chemistry/Computational Modeling Meeting, US Army Corps of Engineers, Vicksburg, MS (presented by Mitchell C. Groenenboom)	Sep. 12, 2017
25.	254th ACS meeting; ENFL division session "Innovative Chemistry & Electrocatalysis for Low-Carbon Energy & Fuels: Discovery to Application", Washington DC	Aug. 22, 2017
24.	Philadelphia Conference in Theoretical Chemistry (PCTC), Philadelphia, PA	Aug. 18, 2017
23.	National Energy Technology Laboratory, Pittsburgh, PA	Apr. 12, 2017
22.	Department of Materials Science and Engineering - Carnegie Mellon University	Feb. 3, 2017
21.	Department of Chemistry and the Center for Photochemical Sciences - Bowling Green State University (BGSU)	Jan. 18, 2017

20.	Department of Chemical and Biomolecular Engineering - Drexel University	Nov. 11, 2016
19.	Army Research Laboratory - Theory department, Aberdeen, MD	Oct. 11, 2016
18.	Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA	Sep. 23, 2016
17.	252th ACS meeting; CATL division session "Electrocatalysis for CO_2 reduction", Philadelphia, PA (presented by Karthikeyan Saravanan)	Aug. 24, 2016
16.	Exploring Chemical Space with Machine Learning and Quantum Mechanics CECAM workshop, ETHZ, Zurich, Switzerland	Jun. 1, 2016
15.	251th ACS National Meeting, ENFL division session "Application of Computational Chemistry for Fuel and Energy Production", San Diego, CA	Mar. 16, 2016
14.	251th ACS National Meeting, CATL division session "Condensed Phase Catalysis Symposium", San Diego, CA	Mar. 15, 2016
13.	I^2CNER International Workshop "CO_2 capture and utilization division", Kyushu University, Fukuoka Japan	Feb. 4, 2016
12.	I^2CNER Annual Symposium "Computational solutions to fundamental problems in carbon-neutral energy research", Kyushu University, Fukuoka Japan	Feb. 1, 2016
11.	2016 Electrochemistry Gordon Research Conference, Ventura, California	Jan. 11, 2016
10.	250th ACS National Meeting, COMP division session "Calculating pKas and Redox Potentials", Boston, MA	Aug. 18, 2015
9.	LONI Institute/LA-SiGMA seminar, Louisiana State University, Baton Rouge, LA	Apr. 1, 2015
8.	ACS Central Regional Meeting 2014, Session: "The Science of CO_2 Capture in Energy Production", Pittsburgh, PA	Oct. 31, 2014
7.	Pitt Center for Simulation and Modeling symposium: "Advancing Research Through High Performance Computing", Pittsburgh, PA	Oct. 15, 2014
6.	248th ACS National Meeting, ENFL division session "Applications of Theoretical Chemistry for Energy and Fuel Production", San Francisco, CA	Aug. 12, 2014
5.	248th ACS National Meeting, PHYS division session "Renewable Energy Generation at the Interface between Theory and Experiment", San Francisco, CA	Aug. 11, 2014
4.	Pittsburgh-Cleveland Catalysis Society, Pittsburgh, PA (presented by Aude Marjolin)	Jun. 02, 2014
3.	247th ACS National Meeting, ENFL division session on Innovations in Carbon Dioxide Capture, Storage, Conversion, and Utilization, Dallas, TX	Mar. 16, 2014
2.	Joint Center for Artificial Photosynthesis (JCAP), Pasadena, CA	Oct. 18, 2013
1.	246th ACS National Meeting, PHYS division session on Solar Energy Conversion, Indianapolis, IN	Sep. 08, 2013

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

37.	232nd ECS Meeting, National Harbor, MD; Galvanic Corrosion of AA7075-T6 Caused By Doped Titanium Oxides in a Controlled Atmospheric Environment (presented by Steven Policastro)	Oct 5, 2017
36. **S**	232nd ECS Meeting, National Harbor, MD; Understanding Electrochemical Reduction of CO_2 Using Quantum Chemistry Modeling (presented by Karthikeyan Saravanan)	Oct 4, 2017
35. **S**	254th ACS meeting, Washington, DC; Deoptimizing oxygen reduction reaction catalysis with doped amorphous Ti oxides (presented by Mitchell C. Groenenboom)	Aug 23, 2017
34. **S**	254th ACS meeting, Washington, DC; Elucidating and correcting the unreliability of continuum solvation methods when modeling homogeneous reaction mechanisms (presented by Yasemin Basdogan)	Aug 22, 2017
33. **S**	25th North American Catalysis Society Meeting, Denver, CO; The mechanism of isobutylene polymerization: new insight into proton-catalyzed polymerizations from the growing string method (presented by Minh Nguyen Vo)	Jun 5, 2017
32. **S**	Pittsburgh Cleveland Catalysis Society, Akron, OH; Accurate computational modeling of chemical reactions in polar solvents using cluster-continuum modeling (presented by Yasemin Basdogan)	May 25, 2017
31.	253rd ACS meeting, San Francisco, CA; Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 coatings for corrosion inhibition	Apr. 6, 2017
30. **S**	16th Annual AIChE, San Francisco, CA; Alloy Catalyst Discovery Using Computational Alchemy (presented by Karthikeyan Saravanan)	Nov. 18, 2016
29. **S**	16th Annual AIChE, San Francisco, CA; First Principles Quantum Chemistry Calculations to Model CO_2 Electroreduction on SnO_2 Particles (presented by Karthikeyan Saravanan)	Nov. 16, 2016
28. **S**	16th Annual AIChE, San Francisco, CA; Neural Network and Reaxff Comparison for Au Properties (presented by Jacob Boes, CMU student)	Nov. 15, 2016
27. **S**	16th Annual AIChE, San Francisco, CA; Comparing the Effect of Counter Ions, Solvent Molecules, and Electron Correlation on Homogeneous Reaction Models (presented by Mitchell C. Groenenboom)	Nov. 15, 2016
26. **S**	Electrochemical Energy Symposium, Pittsburgh, PA; Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 surfaces (presented by Mitchell C. Groenenboom)	Oct. 21, 2016
25. **S**	252th ACS meeting, Philadelphia, PA; Tailoring materials for electrocatalytic reduction of CO_2 (presented by Karthikeyan Saravanan)	Aug. 24, 2016
24. **S**	252th ACS meeting, Philadelphia, PA; Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 surfaces (presented by Mitchell C. Groenenboom)	Aug. 22, 2016
23. **S**	PQI2016, Pittsburgh, PA; Traversing the chemical space - Alloy catalysts discovery using Alchemy (presented by Karthikeyan Saravanan)	Apr. 20, 2016
22. **S**	PQI2016, Pittsburgh, PA; Explicitly unraveling the roles of counter ions and solvent molecules; (Poster presented by Mitchell C. Groenenboom)	Apr. 20, 2016
21.	15th Annual AIChE, Salt Lake City, UT; Liquid Mixtures Freezing at Room Temperature: More Insights into Crystallization and Applications of Poly(trimethylene glycol)/Water Mixtures	Nov. 11, 2015

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

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

18. **S** 228th Electro Chemical Society meeting, Phoenix, AZ; Exploring the non innocence of inorganic complex ligands in (photo)electrochemical CO_2 reduction (presented by Karthikeyan Saravanan) — Oct 11, 2015

17. **S** Science2015 hosted by the Pittsburgh Quantum Institute, Pittsburgh, PA; 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) — Oct. 8, 2015

16. **S** Catalysis in Energy Group Poster Fair, Pittsburgh, PA; 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) — Aug. 11, 2015

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

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

13. **S** 24th North American Catalysis Society Meeting, Pittsburgh, PA; Pourbaix Diagrams of Ruthenium Chromophores Under CO_2 Reduction Conditions; (presented by Karthikeyan Saravanan) — Jun. 16, 2015

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

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

10. **S** 249th ACS National Meeting, Denver, CO; 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) — Mar. 24, 2015

9. 14th Annual AIChE, Atlanta, GA; Water-Induced Crystallization of Poly(trimethyleneglycol); (presented by Robert Enick) — Nov. 19, 2014

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

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

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

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

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

3. **S** 2014 ACS Central Regional Meeting, Pittsburgh, PA; Investigations of nitrogen doping density in graphene and hydrogen adsorption by DFT; (presented by Eric Gottlieb) — Oct. 30, 2014

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

1. **S** 2014 ACS Central Regional Meeting, Pittsburgh, PA; 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) — Oct. 29, 2014

PUBLICATIONS OF WORK DONE AT PITT

[1] Li, P.; Henkelman, G.; Keith, J. A.; Johnson, J. K. Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab initio Molecular Dynamics and Nudged Elastic-Band Studies of $NaBH_4$ Hydrolysis. *J. Phys. Chem. C* **2014**, *118*, 21385–21399, DOI: 10.1021/jp507872d.

[2] Marjolin, A.; Keith, J. A. Thermodynamic Descriptors for Molecules That Catalyze Efficient CO_2 Electroreductions. *ACS Catal.* **2015**, *150*, 1123–1130, DOI: 10.1021/cs501406j.

[3] Grice, K. A.; Groenenboom, M. C.; Manuel, J. D. A.; Sovereign, M. A.; Keith, J. A. Examining the Selectivity of Borohydride for Carbon Dioxide and Bicarbonate Reduction in Protic Conditions. *Fuel* **2015**, *150*, 139–145, DOI: 10.1016/j.fuel.2015.02.007.

[4] Parmelee, S. R.; Mazzacano, T. J.; Zhu, Y.; Mankad, N. P.; Keith, J. A. A Heterobimetallic Mechanism for C-H Borylation Elucidated from Experimental and Computational Data. *ACS Catal.* **2015**, *150*, 3689–3699, DOI: 10.1021/acscatal.5b00275.

[5] Boes, J. R.; Groenenboom, M. C.; Keith, J. A.; Kitchin, J. R. Neural network and ReaxFF comparison for Au properties. *Int. J. Quantum Chem.* **2016**, *116*, 979–987, DOI: 10.1002/qua.25115.

[6] Saravanan, K.; Keith, J. A. Standard redox potentials, pK_as, and hydricities of inorganic complexes under electrochemical conditions and implications for CO_2 reduction. *Dalton Trans.* **2016**, *45*, 15336–15341, DOI: 10.1039/C6DT02371A.

[7] Groenenboom, M. C.; Saravanan, K.; Zhu, Y.; Carr, J. M.; Marjolin, A.; Faura, G. G.; Yu, E. C.; Dominey, R. N.; Keith, J. A. Structural and Substituent Group Effects on Multielectron Standard Reduction Potentials of Aromatic N-Heterocycles. *J. Phys. Chem. A* **2016**, *120*, 6888–6894, DOI: 10.1021/acs.jpca.6b07291.

[8] Groenenboom, M. C.; Keith, J. A. Explicitly Unraveling the Roles of Counterions, Solvent Molecules, and Electron Correlation in Solution Phase Reaction Pathways. *J. Phys. Chem. B* **2016**, *120*, 10797–10807, DOI: 10.1021/acs.jpcb.6b07606.

[9] Saravanan, K.; Gottlieb, E.; Keith, J. A. Nitrogen-doped Nanocarbon Materials Under Electroreduction Operating Conditions and Implications for Electrocatalysis. *Carbon* **2017**, *111*, 859–866, DOI: 10.1016/j.carbon.2016.10.084.

[10] Gray, C. M.; Saravanan, K.; Wang, G.; Keith, J. A. Quantifying solvation energies at solid/liquid interfaces using continuum solvation methods. *Mol. Sim.* **2017**, *43*, 420–427, DOI: 10.1080/08927022.2016.1273525.

[11] Saravanan, K.; Basdogan, Y.; Dean, J. R.; Keith, J. A. Computational investigation of CO_2 electroreduction on tin oxide and predictions of Ti, V, Nb and Zr dopants for improved catalysis. *J. Mater. Chem. A* **2017**, *5*, 11756–11763, DOI: 10.1039/C7TA00405B.

[12] Groenenboom, M. C.; Anderson, R. M.; Horton, D. J.; Basdogan, Y.; Roeper, D. F.; Policastro, S. A.; Keith, J. A. Doped Amorphous Ti Oxides to Deoptimize Oxygen Reduction Reaction Catalysis (**ACS Editors' Choice**). *J. Phys. Chem. C* **2017**, *121*, 16825–16830, DOI: 10.1021/acs.jpcc.7b04210.

[13] Groenenboom, M. C.; Keith, J. A. Quantum Chemical Analyses of BH_4^- and BH_3OH^- Hydride Transfers to CO_2 in Aqueous Solution with Potentials of Mean Force. *ChemPhysChem, accepted* **2017**, *18*, DOI: 10.1002/cphc.201700608.

[14] Kanal, I. Y.; Keith, J. A.; Hutchison, G. R. A Sobering Assessment of Small-Molecule Force Field Methods for Low Energy Conformer Predictions. *Int. J. Quantum Chem., accepted* **2017**, DOI: 10.1002/qua.25512.

[15] Vo, M. N.; Bryantsev, V. S.; Johnson, J. K.; Keith, J. A. Quantum Chemistry Benchmarking of Binding and Selectivity for Lanthanide Extractants. *Int. J. Quantum Chem., accepted* **2017**, DOI: 10.1002/qua.25516.

PUBLICATIONS OF WORK DONE BEFORE ARRIVING AT PITT

[1] Keith, J. A.; Oxgaard, J.; Goddard III, W. A. Inaccessibility of β-hydride Elimination From -OH Functional Groups in Wacker–type Oxidation. *J. Am. Chem. Soc.* **2006**, *128*, 3132–3133, DOI: 10.1021/ja0533139.

[2] Keith, J. A.; Behenna, D. C.; Mohr, J. T.; Ma, S.; Marinescu, S. C.; Oxgaard, J.; Stoltz, B. M.; Goddard III, W. A. The Inner-sphere Process in the Enantioselective Tsuji Allylation Reaction with (S)-t-Bu-phosphinooxazoline Ligands. *J. Am. Chem. Soc.* **2007**, *129*, 11876–11877, DOI: 10.1021/ja070516j.

[3] Keith, J. A.; Nielsen, R. J.; Oxgaard, J.; Goddard III, W. A. Unraveling the Wacker Oxidation Mechanisms. *J. Am. Chem. Soc.* **2007**, *129*, 12342–12343, DOI: 10.1021/ja072400t.

[4] Lu, J.-Y.; Keith, J. A.; Shen, W.-Z.; Schürmann, M.; Preut, H.; Jacob, T.; Arndt, H.-D. Regioselective De Novo Synthesis of Cyanohydroxypyridines with a Concerted Cycloaddition Mechanism. *J. Am. Chem. Soc.* **2008**, *130*, 13219–13221, DOI: 10.1021/ja804078v.

[5] Keith, J. A.; Henry, P. M. The mechanism of the Wacker reaction: a tale of two hydroxypalladations. *Angew. Chem. Int. Ed.* **2009**, *48*, 9038–9049, DOI: 10.1002/anie.200902194.

[6] Keith, J. A.; Nielsen, R. J.; Oxgaard, J.; Goddard III, W. A.; Henry, P. M. Comment on "Mechanism and Kinetics of the Wacker Process: A Quantum Mechanical Approach". *Organometallics* **2009**, *28*, 1618–1619, DOI: 10.1021/om800013p.

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