

**Eric A. Walker**

Computational and Data-Enabled Science and Engineering  
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## CURRICULUM VITAE

### RESEARCH INTERESTS

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- Computational catalysis
- Oxide materials
- Interface catalysis
- Data science

### EDUCATION

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- **Ph.D. Chemical Engineering** [August 2016]  
University of South Carolina (USC)-Columbia, SC  
Thesis Title: Uncertainty Quantification in Computational Catalysis  
Advisor: Dr. Andreas Heyden, Co-advisor: Dr. Gabriel A. Terejanu (Computer Science)
- **M.S. Chemical Engineering** [December 2013]  
University of South Carolina (USC)-Columbia, SC  
Thesis Title: Comparison of a Particle Filter and Other State Estimation Methods for Prognostics of Lithium-Ion Batteries.  
Thesis available at <http://scholarcommons.sc.edu/etd/2565>  
Advisor: Dr. Ralph E. White
- **B.S. Chemical & Biomolecular Engineering** [December 2009]  
Georgia Institute of Technology-Atlanta, GA

### HONORS AND AWARDS

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- Presidential fellowship- \$32,000 financial support from the University of South Carolina, USC's most prestigious university-wide award for promise of excellence at the graduate level, nomination from the graduate director, presented "work in progress" 3<sup>rd</sup> year.
- 2014 Eastman Fellowship- \$5000 financial support from Eastman Chemical Co., awarded for outstanding graduate academic research accomplishments in the area of heterogeneous catalysis, presented research at Eastman Headquarters Kingsport, TN.
- Best Paper- Data Driven Screening of Chemical and Materials Space session AIChE Annual Meeting 2018
- Institute for Mathematics and its Applications- fully paid two week short course "Introduction to Uncertainty Quantification" at the University of Minnesota
- Two time travel award (Gordon Research Conference Catalysis 2014 and AIChE Annual Meeting 2014 Atlanta, GA) from the Graduate Office, USC.
- Catalysis Reaction Engineering Division Travel Award (AIChE Annual Meeting Salt Lake City, UT 2015).

- American Chemical Society (ACS) Catalysis Division registration waiver (ACS spring meeting 2016 San Diego, CA).
- Oral presentation award third place student (Southeastern Catalysis Society Asheville, NC fall 2014).
- Tau Beta Pi, Highest Honors (Georgia Institute of Technology).
- HOPE Scholarship- State of Georgia paid tuition and fees for Bachelor of Science degree.

## PROFESSIONAL EXPERIENCE

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- **Research Assistant Professor** [January 2019-present]
- Research area and teaching: Conducted research in areas of computational data sciences including topics in computational catalysis, uncertainty quantification, Bayesian statistical tools, high performance computation, and machine learning. Developed training modules that result in badges and micro-credentials in the area of computational and data science. Taught Data Intensive Python.  
Original modules developed: Bayesian Design of Experiments: Part #1, Linear Algebra at Scale.  
Institute for Computational and Data Sciences  
Adjunct appointment- Chemical and Biological Engineering since January 2020  
University at Buffalo, the State University of New York  
Institute Director- Dr. Abani Patra
- **Postdoctoral Fellow** [September 2016-December 2018]  
Topic: Applying novel machine learning techniques to chemical challenges in materials and catalyst optimization. Learning to predict reaction conditions: relationships between solvent and catalyst.  
University of Michigan-Ann Arbor, Department of Chemistry  
Postdoctoral mentor- Dr. Paul Zimmerman
- **Research Assistant** [May 2011-August 2016]  
University of South Carolina, Department of Chemical Engineering  
Research area: Uncertainty Quantification in Computational Catalysis.  
Programmed microkinetic models into the library Quantification of Uncertainty for Estimation, Simulation and Optimization (QUESO). Assisted in the implementation of adsorbate-adsorbate interactions for surface-catalyzed reactions. Programming languages: C++, Linux, version control (Git), MATLAB, Materials Studio, and others.

- **Systems Support Engineer** [January 2010- February 2011]  
Savannah River Nuclear Solutions, LLC, Aiken, SC  
Supported and oversaw the Department of Energy Safety Basis Implementation for the High Activity Waste system in H-Canyon, a robust, highly shielded nuclear processing facility which separates nuclear materials.
- **Co-op- Cryogenics**  
Air Products & Chemicals, Inc., Allentown, PA [May-August 2008]  
Tracked, managed, and interpreted data from Air Separation plant.  
Gained knowledge of cryogenic distillation.
- **Co-op- International Space Station Procurement**  
NASA Johnson Space Center, Houston, TX [August-December 2006]  
Applied Government contract processes.

## TEACHING EXPERIENCE

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- Module Bayesian Design of Experiments: Part #1- Conceived course and created content including lecture slides, assignments, and solutions. Taught to industry professionals and graduate students representing a variety of industries and disciplines, respectively.
- Module Linear Algebra at Scale- Generated course content and taught.
- Module Data Intensive Python- Taught and expanded multivariate regression portion.
- Kinetics (ECHE 430) two semesters- lectured to students, graded exams and homeworks, led computer lab sessions, prepared homework solutions.  
Biomedical Engineering Principles (BMEN 211)- led computer lab sessions.  
Fluid mechanics (ECHE 320) - graded homeworks.  
Graduate chemical process analysis (ECHE 700)- graded homeworks, prepared homework solutions.  
Graduate chemical reactor design (ECHE 730)- graded homeworks, prepared homework solutions. Software used in teaching- MATLAB, Microsoft Office, COMSOL, Maple and others. [August 2011-August 2016]

## STUDENTS MENTORED

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- Kishore Ravisankar, M. S. Data Science, University at Buffalo, February 2020, employed from March 2020 with HCL Technologies, Inc., contractor for Ford Motor Co., Dearborn, MI
- Kevin Giewont (co-advised), M. S. Chemical and Biological Engineering, University at Buffalo (expected)

- Caitlin Horvatits (co-advised), M. S. Chemical and Biological Engineering, University at Buffalo, May 2020 (expected)
- Timothy Buchanan (co-advised), B. S. Chemical and Biological Engineering (expected), University at Buffalo
- Guided computational project of Mohammadmoein Mohammadi, Ph.D. candidate Chemical and Biological Engineering, University at Buffalo
- Donald Mitchell, B. S. City College of New York, Research Experience for Undergraduates (REU), University of South Carolina [May-August 2014]

## JOURNAL PUBLICATIONS

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1. Horvatits, C.; Li, D.; Dupuis, M.; Kyriakidou, E. A.; **Walker, E. A.** Ethylene and Water Co-Adsorption on Ag/SSZ-13 Zeolites: A Theoretical Study. **2020** *accepted J. Phys. Chem. C.*, 10.1021/acs.jpcc.0c00849.
2. Kammeraad, J.; Goetz, J.; **Walker, E.**; Tewari, A.; Zimmerman, P. What Does the Machine Learn? **2020** *accepted J. Chem. Inf. Model*, 10.1021/acs.jcim.9b00721.
3. **Walker, E.**; Ravisankar, K. Bayesian Design of Experiments: Implementation, Validation and Application to Chemical Kinetics. **2019** arXiv:1909.03861.
4. **Walker, E.**; Kammeraad, J.; Goetz, J.; Robo, M.; Tewari, A.; Zimmerman, P. Learning to Predict Reaction Conditions: Relationships between Solvent, Reactants and Catalyst. *J. Chem. Inf. Model.* **2019**, 59 (9), 3645-3654.
5. Chowdhury, A.; Yang, W.; **Walker, E.**; Mamun, O.; Heyden, A.; Terejanu, G. Prediction of Adsorption Energies for Chemical Species on Metal Catalyst Surfaces Using Machine Learning. *J. Phys. Chem. C.* **2018**, 122 (49), 28142-28150. Selected as Editor's Choice- Editor's Choice- due to its potential for broad public interest, an honor given to only one article from the entire American Chemical Society portfolio each day.
6. **Walker, E.**; Mitchell, D.; Terejanu, G. A.; Heyden, A. Identifying Active Sites of the Water-Gas Shift Reaction over Titania Supported Platinum Catalysts under Uncertainty. *ACS Catal.* **2018**, 8, 3990-3998.
7. Mamun, O.; **Walker, E.**; Faheem, M.; Bond, J. Q.; Heyden, A. Theoretical Investigation of the Hydrodeoxygenation of Levulinic Acid over Ru (0001): A DFT and Microkinetic Modeling Study. *ACS Catal.* **2017**, 7, 215-228.

8. **Walker, E.**; Terejanu, G. A.; Ammal, S. C.; Heyden, A. Uncertainty Quantification Framework Applied to the Water-Gas Shift Reaction over Pt-based Catalysts. *J. Phys. Chem. C* **2016**, 120, 10328-10339.
9. Behtash, S.; Lu, J.; **Walker, E.**; Mamun, O.; Heyden, A. Solvent Effects in the Liquid Phase Hydrodeoxygenation of Methyl Propionate over a Pd (111) Catalyst Model. *J. Catal.* **2016**, 333, 171-183.
10. **Walker, E.**; Rayman, S.; White, R. E. Comparison of a Particle Filter and Other State Estimation Methods for Prognostics of Lithium-ion Batteries. *J. Power Sources* **2015**, 287, 1-12.
11. **Walker, E.**; Ammal, S. C.; Suthirakun, S.; Chen, F.; Terejanu, G. A.; Heyden, A. Mechanism of Sulfur Poisoning of Sr<sub>2</sub>Fe<sub>1.5</sub>Mo<sub>0.5</sub>O<sub>6-δ</sub> Perovskite Anode under Solid Oxide Fuel Cell Conditions. *J. Phys. Chem. C* **2014**, 118, 23545-23552.
12. **Walker, E.**; Terejanu, G. A.; Ammal, S. C.; Heyden, A. Uncertainty Quantification of the Water-Gas Shift Reaction over Pt/CeO<sub>2</sub> Catalyst. Under preparation.

## INVITED LECTURES

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- "Data Science in Computational Catalysis" **Walker, E.** Department of Chemical and Biological Engineering, University at Buffalo [February 2020]
- "Data Science in Computational Catalysis" **Walker, E.** Chemical and Biomolecular Engineering Department, Clarkson University, Potsdam, NY [January 2020]
- "Atomic Simulation and Data Science Applied to Catalysis" **Walker, E.** School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK [February 2019]

## ORAL PRESENTATIONS

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- "Trapping Properties of Ag/SSZ-13 Zeolite: Modeling Adsorption Capacity" **Walker, E.**; Horvatits, C. A.; Li, D.; Dupuis, M.; Kyriakidou, E. A. American Institute of Chemical Engineers Annual Meeting Orlando, FL [November 2019]
- "Uncertainty Quantification of the Water-Gas Shift Reaction by Pt/CeO<sub>2</sub> Catalyst" **Walker, E.**; Terejanu, G. A.; Ammal, S. C.; Heyden, A. American Institute of Chemical Engineers Annual Meeting Orlando, FL [November 2019]
- "Data Science in Computational Catalysis" **Walker, E.** Brookhaven National Laboratory [February 2019]
- "Connecting Experimental Conditions with Chemical Structure" **Walker, E.**; Kammeraad, J.; Goetz, J.; Tewari, A.; Zimmerman, P. M. American Institute of Chemical Engineers annual meeting Pittsburgh, PA. Voted best paper in Data-Driven Screening of

- Chemical and Materials Space [October 2018]
- “Reaction Path Discovery Under Potential Bias” **Walker, E.**; Jafari, M.; Zimmerman, P. M. American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN [November 2017]
  - “Explaining Surface-Catalyzed Reactions in Electrochemistry” **Walker, E.** American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN [October 2017]
  - “Uncertainty Quantification of the Water-Gas Shift Reaction by Pt/CeO<sub>2</sub> Catalyst” **Walker, E.**; Ammal, S. C.; Terejanu, G. A.; Heyden, A. American Institute of Chemical Engineers Annual Meeting, San Francisco, CA [November 2016]
  - “Correlating Experimental Data with Computational Models for Active Site Model Identification: A Case Study for the Water-Gas Shift Reaction” Heyden, A.; **Walker, E.**; Terejanu, G. A.; Ammal, S. C. American Chemical Society Spring Meeting, San Diego, CA [March 2016]
  - “Uncertainty Quantification of the Water-Gas Shift Reaction over Pt-Based Catalysts” **Walker, E.**; Terejanu, G. A.; Ammal, S. C.; Heyden, A. American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT [November 2015]
  - “Uncertainty Quantification of the Water-Gas Shift Reaction over Pt-Based Catalysts” **Walker, E.**; Terejanu, G. A.; Ammal, S. C.; Heyden, A. Advances in Computing graduate seminar Department of Computer Science University of South Carolina [fall 2015]
  - “DFT Uncertainty Quantification of the Water-Gas Shift Reaction over Pt-Based Catalysts” **Walker, E.**; Terejanu, G. A.; Heyden, A. Oak Ridge National Laboratory main campus [summer 2015]
  - “Uncertainty Quantification of the Water-Gas Shift Reaction over Pt-Based Catalysts” **Walker, E.**; Terejanu, G. A.; Heyden, A. Fuels, Engines and Emissions Research Center, Oak Ridge National Laboratory Knoxville, TN [summer 2015]
  - “Theoretical Investigation of H<sub>2</sub> and CO Electro-Oxidation on the Sr<sub>2</sub>Fe<sub>1.5</sub>Mo<sub>0.5</sub>O<sub>6-d</sub>(001) Perovskite Surface Under Anodic Solid Oxide Fuel Cell Conditions” Ammal, S. C.; Suthirakun, S.; **Walker, E.**; Heyden, A. North American Catalysis Society Meeting Pittsburgh, PA [June 2015]
  - “Uncertainty Quantification of Computational Catalysis” **Walker, E.** University of South Carolina graduate student day [spring 2015]
  - “Uncertainty Quantification of a Computational Study of the Water-Gas Shift Reaction Catalyzed By Platinum Clusters Supported on Titanium Oxide (Pt/TiO<sub>2</sub>)” **Walker, E.**; Terejanu, E. A.; Ammal, S. C.; Heyden, A. American Institute of Chemical Engineers Annual Meeting, Atlanta, GA [fall 2014]
  - “Combined DFT and Microkinetic Modeling of H<sub>2</sub> and CO Electrooxidation on the Sr<sub>2</sub>Fe<sub>1.5</sub>Mo<sub>0.5</sub>O<sub>6-d</sub>(001) Perovskite Anode” Ammal, S. C.; Suthirakun, S.; **Walker, E.**;

Heyden, A. American Institute of Chemical Engineers Annual Meeting Atlanta, GA  
[November 2014]

- “Uncertainty Quantification of Computational Catalysis Studies” **Walker, E.** Eastman Chemical Company Research Division Kingsport, TN [fall 2014]
- “Uncertainty Quantification of a Computational Study of the Water-Gas Shift Reaction Catalyzed by Platinum Clusters Supported on Titanium Oxide (Pt/TiO<sub>2</sub>)” **Walker, E.;** Terejanu, E. A.; Ammal, S. C.; Heyden, A. Southeastern Catalysis Society Meeting Asheville, NC [September 2014]

## POSTER PRESENTATIONS

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- “Reaction Path Discovery under Potential Bias” **Walker, E.;** Zimmerman, P. M. Michigan Institute for Computational Discovery and Engineering Ann Arbor, MI [March 2017]
- “Rational Design of Catalytic Materials for Advancing the Use of Alternative Energy Sources” **Walker, E.** American Institute of Chemical Engineers San Francisco, CA [November 2016]
- “Determination of the Active Site of the Water-Gas Shift Reaction over Pt/TiO<sub>2</sub> Catalyst” **Walker, E.;** Terejanu, E. A.; Ammal, S. C.; Heyden, A. American Chemical Society Meeting San Diego, CA [March 2016]
- “Theoretical Study of the Reaction Mechanism and Structure Sensitivity of the Hydrodeoxygenation of Propanoic Acid over Pd Catalysts in Vapor and Liquid Phase Environments” **Walker, E.;** Solomon, R. V.; Behtash, S.; Heyden, A. American Chemical Society Meeting San Diego, CA [March 2016]
- “Uncertainty Quantification in Computational Catalysis” **Walker, E.;** Terejanu, E. A.; Ammal, S. C.; Heyden, A. Center for Rational Catalyst Synthesis (CERCAS) University of South Carolina [spring 2015]
- “Uncertainty Quantification in Computational Catalysis” Mitchell, D.; **Walker, E.;** Heyden, A. American Institute of Chemical Engineers Annual Meeting Atlanta, GA [November 2014]

## PROFESSIONAL SERVICE

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- Session Chair, New Developments in Computational Catalysis American Institute of Chemical Engineers Annual Meeting, Orlando, FL [November 2019]
- National Science Foundation proposal review panel [spring 2019]
- Session Chair, New Developments in Computational Catalysis II American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA [October 2018]
- Session Chair, Fundamentals of Surface Reactivity American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN [November 2017]

- Session Co-Chair, New Developments in Computational Catalysis American Institute of Chemical Engineers Annual Meeting, Minneapolis, MN [October 2017]
- Session Co-Chair, Fundamentals of Surface Reactivity II American Institute of Chemical Engineers Annual Meeting, San Francisco, CA [November 2016]
- Chemical Engineering Graduate Student Organization technology chair (website), University of South Carolina [fall-spring 2012]

## **SOCIETY MEMBERSHIPS**

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- American Institute of Chemical Engineers
- American Chemical Society
- Tau Beta Pi

## **PROPOSAL WRITING**

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Contributed preliminary results to NSF-DMREF 1534260 awarded \$840,000 (September 2015): Collaborative Research: Design and Discovery of Multimetallic Heterogeneous Catalysts for a Future Biorefining Industry