
CURRICULUM VITAE

NAME: ADITYA SAVARA **CITIZENSHIP:** US

AFFILIATIONS: STAFF SCIENTIST, OAK RIDGE NATIONAL LAB
ADJUNCT PROFESSOR, VIRGINIA TECH (MAT. SCI. & ENG.)

PROFILE

Heterogeneous catalysis, chemical kinetics, data science, complex reaction mechanisms, chemistry of surfaces: simulations, vibrational spectroscopy, energy applications, environmental applications.

2003-2008 Ph.D. in Physical Chemistry, Northwestern University **Evanston, IL**

2000-2003 B.S. in Chemistry, University of Hawaii **Honolulu, HI**

RESEARCH EXPERIENCE

2011–Present Kinetics and Catalysis (Staff), ORNL **Oak Ridge, TN**

- Conversion of organic oxygenates over Oxides; including Ethanol to Hydrogen, Acetone, and Ethanal. Experiments and Kinetic simulations. (*1 Patent Expected*)
- Project Leader for software Kinetic Monte Carlo of Systems (KMCOS), for modeling reactions of molecular species on surfaces.
- Primary Author of CheKiPEUQ Software, which uses Bayesian Parameter Estimation (data science) for more physically realistic matches between experiment and predictions, based on experimental and theoretical uncertainties. (*1 Cover Feature*)
- Atomic scale to reactor scale (State-of-the-Art) multiscale modeling using Kinetic Monte Carlo and Fluid Dynamics simulations (catalytic CO oxidation over RuO₂).
- Elucidation of the kinetics and mechanism in benzylic alcohol oxidation over Pd and AuPd nanoparticles for greener alcohol oxidation. (*2 Inside Journal Covers*)
- Infrared discovery of aromatic-hydroxyl interactions for BPEa-SBA-15, a lignin model compound, with the interaction present at pyrolysis temperatures. (*Inside Journal Cover*)

2008–2011 Freund Group, Fritz Haber Institute **Berlin, Germany**

- Role of subsurface hydrogen in the selectivity of isomerization and hydrogenation of *cis*-2-butene over Pd nanoparticles and Pd(111).
- Non Langmuir-Hinshelwood kinetics for H/D exchange over Pd nanoparticles and Pd(111): Interpreted as subsurface hydrogen combining with surface hydrogen via a “breakthrough” mechanism to form H₂/D₂/HD. (*Featured as Editor’s Choice*)

2003–2008 Weitz Group, Northwestern University **Evanston, IL**

- Reaction kinetics of NO_x reduction over Ba-Y zeolites and related catalysts.
- First observation that nanoscale pores can alter a reaction mechanism.
- Discovered the acid catalyzed reduction of NH₄NO₃ by NO
- Enthalpies and entropies of gas adsorption on surfaces, a theoretical investigation.

2002–2003 Jensen Group, University of Hawaii **Honolulu, HI**

- Catalyzed dehydrogenation of sodium aluminum hydride by titanium doping.

TEACHING EXPERIENCE

- 2003–2004 Northwestern University** **Evanston, IL**
- 2003 & 2004 Chem 333L: Inorganic Chemistry TA
 - 2004 Chem 172L: Accelerated Physical Chemistry TA
 - 2003 Chem 171L: Accelerated Inorganic Chemistry TA

AWARDS & RECOGNITION

- 2020 White House Fellows Program - Regional Finalist
- 2007 ACS Graduate Student Award in Environmental Chemistry
- 2004 Keynote Speaker for NU New Teaching Assistants Luncheon (College-wide)
- 2004 NU WCAS Outstanding Graduate Student Teacher Award (College-wide)
- 2004 PLU L. Carroll King Award for Excellence in 100-Level Teaching (Department)

LEADERSHIP & SERVICE

- 2021-Present ACS Division Activities Committee (*National*)
- 2018-Present ACS Catalysis Division Councilor
- 2017-Present ACS Multidisciplinary Program Planning Group (*National*)
- 2020 ACS Meetings and Expositions Committee (*National*)
- 2017-2019 ACS Catalysis Division Spring Program Chair
- 2016-2019 ACS Environmental Division Membership Chair
- 2012-2015 ACS Environmental Division Secretary
- 2004-2008 Northwestern University Graduate Leadership Council
- 2006-2007 Northwestern University Graduate Student Association President
- 2004-2006 Northwestern University Graduate Student Association VP

SELECTED FUNDING AWARDED

- ORNL DOE LDRD project ID: 9824. Controlling Reversibility in Next-Generation Upcycling Polymers. **2019-2021. \$1,600,000.** Co-PI.
- DOE BES Catalysis Science: ERKC96. Fundamentals of Catalysis and Chemical Transformations. **2017-2020 \$6,867,000.** Co-PI.
- ORNL DOE LDRD SEED project ID: 8729 Experimental Data Based Combinatorial Kinetic Simulations for Predictions of Enhanced Exhaust Emission Catalysis. **2017-2018 \$190,000.** PI.
- ORNL DOE LDRD project ID: 7427 Predictive computational catalysis: From electrons to reactors. **2015-2017 \$1,159,000.** PI.
- ORNL DOE LDRD project ID: 6895 Sustainable Energy through Complex Oxide Materials: Multivalent Oxygen Sponges for Efficient, Low Temperature Catalysts. **2013-2015 \$395,000.** Co-PI.
- ORNL DOE LDRD project ID: 6584 Elucidating & Developing Spillover Catalysis: A New Paradigm for Predictive Catalysis. **2011-2013 \$675,000.** PI.

Publications, Service, Mentoring, for Aditya Savara

55 Journal Articles, h-index of ~20

A) Journal Articles

1. Chen, B.; Xu, Y.; Xiong, C.; Rickard, S.; Boscoboinik, J.; Jiang, D.-e.; Kidder, M.; **Savara, A.**, Mechanism for Acetone and Crotonaldehyde Production during Steam Reforming of Ethanol over La_{0.7}Sr_{0.3}MnO_{3-x} Perovskite: Evidence for a Shared C₄ Aldol-Addition Intermediate. *ACS Catalysis* **2022**, *12*, 4358.
2. Md. Rahman, C. Bowland, S. Ge, S. R. Acharya, S. Kim, V. R. Cooper, X. Chen, S. Irle, A. Sokolov, **A. Savara** and T. Saito. “Design of tough adhesive from commodity thermoplastics through dynamic crosslinking”. *Science Advances*, **2021**, *7*, eabk2451.
3. Chen, B.; Xiong, C.; Jiang, D.-e.; **Savara, A.*** “Ethanol Conversion over La_{0.7}Sr_{0.3}MnO_{3-x}(100): Autocatalysis, Adjacent O-Vacancies, Disproportionation, and Dehydrogenation.” *ACS Catalysis* **2020**, *10*, 12920-12931.
4. Walker, E. A.; Ravisankar, K.; **Savara, A.** “Chekipeuq Intro 2: Harnessing Uncertainties from Data Sets, Bayesian Design of Experiments in Chemical Kinetics.” *ChemCatChem* **2020**, *12*, 5401-5410.
5. **Savara, A.***; Walker, E. A. “Chekipeuq Intro 1: Bayesian Parameter Estimation Considering Uncertainty or Error from Both Experiments and Theory.” *ChemCatChem* **2020**, *12*, 5385-5400.
**Cover Feature ([link to feature](#))
6. Wu, P; Tan, S; Moon, J; Yan, Z; Fung, V; Li, N; Yang, S-Z; Cheng, Y; Abney, CW; Wu, Z; **Savara, A**; Momen, AM; Jiang, D; Su, D; Li, H; Zhu, W; Dai, S; Zhu, H. “Harnessing strong metal–support interactions via a reverse route.” *Nat. Comm.*, **2020**, *11*, 3042. doi:10.1038/s41467-020-16674-y
7. Zhang, X.; **Savara, A.***; Getman, R. B. “A Method for Obtaining Liquid–Solid Adsorption Rates from Molecular Dynamics Simulations: Applied to Methanol on Pt(111) in H₂O” *JCTC*, **2020**, *16*, 2680-2691.
**Supplemental Cover ([link to image](#))
8. Doyle, P.J.; **Savara, A.***; Raiman, S.S. “Extracting Meaningful Standard Enthalpies and Entropies of Activation for Surface Reactions from Kinetic Rates”, *React. Kinet. Mech. Cat.*, **2020**, *129*, 551-581.
9. Zhang, Y.; Mullins, D.R.; **Savara, A.*** “Surface Reactions and Catalytic Activities for Small Alcohols over LaMnO₃(100) and La_{0.7}Sr_{0.3}MnO₃(100):

- Dehydrogenation, Dehydration, Oxidation.” *J. Phys. Chem. C.*, **2020**, *124*, 3650-3663.
10. **Savara, A.*** “Microkinetic Simulation and Fitting of the Temperature Programmed Reaction of Methanol on CeO₂(111): H₂ and H₂O + V Production.” *React. Kinet. Mech. Cat.*, **2020**, *129*, 181-203.
 11. Matera, S.; Schneider, W. F.; Heyden, A.; **Savara, A.*** “Progress in Accurate Chemical Kinetic Modeling, Simulations, and Parameter Estimation for Heterogeneous Catalysis.” *ACS Catalysis*, **2019**, *9* (8), 6624-6647.
****Invited Perspective**
 12. Vuong, H.; Binder, A. J.; Sutton, J. E.; Toops, T.; **Savara, A.*** Experimental Data Based Combinatorial Kinetic Simulations for Predictions of Synergistic Catalyst Mixtures. *Catal Today*, **2019**, *338*, 117-127. 10.1016/j.cattod.2019.04.026
****Invited Article**
 13. Zhang, Y.; Mullins, D.R.; **Savara, A.*** "Effect of Sr Substitution in LaMnO₃(100) on Catalytic Conversion of Acetic Acid to Ketene and Combustion-like Products" *J. Phys Chem. C.* **2019**, *123*, 4148-4157.
 14. Zhao, C.; Watt, C.; Kent, P.; Overbury, S.H.; Mullins, D.R.; Calaza, F.C.; **Savara, A.***; Xu, Y. "Coupling of acetaldehyde to crotonaldehyde on CeO_{2-x}(111): Bifunctional mechanism and role of oxygen vacancies" *J. Phys Chem. C.* **2019**, *123* (13), 8273-8286.
****Invited Article**
 15. Chan-Thaw CE, **Savara A**, Villa A.; Selective Benzyl Alcohol Oxidation over Pd Catalysts. *Catalysts*, **2018**, *8*, 431.
****Invited Review**
 16. Liu, C.; Camacho-Bunquin, J.; Ferrandon, M.; **Savara, A.**; Sohn, H.; Yang, D.; Kaphan, D. M.; Langeslay, R. R.; Ignacio-de Leon, P. A.; Liu, S., et al. Development of Activity-Descriptor Relationships for Supported Metal Ion Hydrogenation Catalysts on Silica. *Polyhedron*, **2018**, *152*, 73-83.
 17. Nellis, C.; Danielson, T.; **Savara, A.**; Hin, C. “The F-t-Pj-RG method: An Adjacent-Rolling-Windows Based Steady-State Detection Technique for Application to Kinetic Monte Carlo Simulations” *Comp Phys Comm*, **2018**, *232*, 124.
 18. **Savara, A.**; Sutton, J. “SQERT-T: alleviating KMC-stiffness in transient kinetic Monte Carlo simulations.” *J. Phys. Cond. Matt.*, **2018**, *30*, 295901. 10.1088/1361-648X/aacb6d
****Invited Article**

19. Nellis, C.; Hin, C.; **Savara, A.** “The ϕ -Relation and a Simple Method to Predict How Many Data Points Are Needed for Relevant Steady-State Detection.” *AIChE*, **2018**, *64*, 3354.
20. Sutton, J.E.; Lorenzi, J.M.; Krogel, J.; Xiong, Q.; Pannala, S.; Matera, S.; **Savara, A.*** “Electrons to Reactors Multiscale Modeling: Catalytic CO Oxidation over RuO₂” *ACS Catalysis* **2018**, *8*, 5002-5016.
21. Prati, L.; Villa, A.; Jouve, A.; Beck, A.; Evangelisti, C.; **Savara, A.** “Gold as Modifier of Metal Nanoparticles: Effect on Structure and Catalysis.” *Faraday Discussions* **2018**, *208*, 395-407. DOI: 10.1039/C7FD00223H
22. Sutton, J.E.; Danielson, T.; Beste, A.; **Savara, A.*** “Below-Room-Temperature C–H Bond Breaking on an Inexpensive Metal Oxide: Methanol to Formaldehyde on CeO₂(111)” *J. Phys. Chem. Lett.*, **2017**, *8*, 5810–5814.
DOI: 10.1021/acs.jpcclett.7b02683
** **ACS LiveSlides**: <https://pubs.acs.org/doi/suppl/10.1021/acs.jpcclett.7b02683>
23. Zhang, Y.; **Savara, A.**; Mullins, D. “Ambient-Pressure XPS Studies of Reactions of Alcohols on SrTiO₃(100)” *J. Phys Chem. C*, **2017**, *121*, 23436–23445.
24. W. Liu; Y. Jiang; K.-H. Dostert; C. P. O'Brien; W. Riedel; **A. Savara**; S. Schauermaun and A. Tkatchenko; "Catalysis beyond frontier molecular orbitals: Selectivity in partial hydrogenation of multi-unsaturated hydrocarbons on metal catalyts." *Sci. Adv.* **2017**. DOI: 10.1126/sciadv.1700939
25. **Savara, A.** Correction to “Comment on ‘Equilibrium Constants and Rate Constants for Adsorbates: 2D Ideal Gas, 2D Ideal Lattice Gas, and Ideal Hindered Translator Models’” *J. Phys. Chem. C*, **2017**, *121*, 14990.
10.1021/acs.jpcc.7b05171
26. Danielson, T.; Sutton, J.; Hin, C.; **Savara, A.** “SQERTSS: Dynamic Rank Based Throttling of Transition Probabilities in Kinetic Monte Carlo Simulations” *Comp Phys Comm*, **2017**, *216*, 149. <https://doi.org/10.1016/j.cpc.2017.05.016>
27. **Savara, A.**; Chan-Thaw, C.E.; Sutton, J.E.; Wang, D.; Prati, L.; Villa, A. “Molecular Origin of Selectivity Differences Between Pd and AuPd in Benzyl Alcohol Oxidation: Different Oxygen Adsorption Properties” *ChemCatChem*, **2017**, *9*, 253. DOI: 10.1002/cctc.201601295
****Featured Article, Inside Cover / Back Cover** (10.1002/cctc.201700009)
28. **Savara, A.** “Comment on Equilibrium Constants and Rate Constants for Adsorbates: Two-Dimensional (2D) Ideal Gas, 2D Ideal Lattice Gas, and Ideal Hindered Translator Models” *J. Phys Chem. C*, **2016**, *120*, 20478. DOI: 10.1021/acs.jpcc.6b07553

29. Danielson, T.; Hin, C.; **Savara, A.** “Generalized Adsorption Isotherms for Molecular and Dissociative Adsorption of a Polar Molecular Species on Two Polar Surface Geometries: Perovskite (100) (Pm-3m) and Fluorite (111) (Fm-3m)” *J. Chem. Phys.*, **2016**, *145*, 064705. <http://dx.doi.org/10.1063/1.4960508>
30. **Savara, A.** “Simulation and Fitting of Complex Reaction Network TPR: The Key Is The Objective Function” *Surf Sci*, **2016**, *653*, 169. DOI: 10.1016/j.susc.2016.07.001
31. **Savara, A.**; Rossetti, I.; Chan-Thaw, C.E.; Prati, L.; Villa, A. “Microkinetic Modeling of Benzyl Alcohol Oxidation on Carbon Supported Pd Nanoparticles” *ChemCatChem*, **2016**, *8*, 2482. DOI: 10.1002/cctc.201600368
**Featured Article, and Inside Cover
32. K.-H. Dostert; C. P. O'Brien; W. Liu; W. Riedel; **A. Savara**; A. Tkatchenko; S. Schauermaun and H.-J. Freund. "Adsorption of isophorone and trimethylcyclohexanone on Pd(111): A combination of infrared reflection absorption spectroscopy and density functional theory studies." *Surf Sci.* **2016**.
doi:10.1016/j.susc.2016.01.026
33. Gur, S.; Danielson, T.; Xiong, Q.; Hin, C.; Pannala, S.; Frantziskonis, G.; **Savara, A.**; Daw, C.S. “Wavelet-based surrogate time series for multiscale simulation of heterogeneous catalysis” *Chem Eng Sci*, **2016**
<http://dx.doi.org/10.1016/j.ces.2016.01.037>.
34. **Savara, A.**; Chan-Thaw, C.E.; Rossetti, I.; Villa, A.; Prati, L. “Benzyl Alcohol Oxidation on Carbon Supported Pd Nanoparticles: Elucidating the Reaction Mechanism” *ChemCatChem*, **2014**, *6*, 3464-3473. DOI: 10.1002/cctc.201402552
35. Kandziolka, M.V.; Kidder, M.K.; Gill, L.; Wu, Z.; **Savara, A.** “Aromatic-Hydroxyl Interaction of an alpha-aryl ether Lignin Model-Compound on SBA-15, Present at Pyrolysis Temperatures” *PCCP*, **2014**, *16*, 24188 - 24193. DOI: 10.1039/C4CP02633K
**Featured Article, and Back Cover ([link](#))
36. Dostert, K.-H.; O'Brien, C.P.; Ridel, W.; **Savara, A.**; Liu, W.; Oehzelt, M.; Tkatchenko, A.; Schauermaun, S. “Interaction of Isophorone with Pd(111): A Combination of IRAS, NEXAFS and DFT Studies” *J. Phys. Chem.*, **2014**, *118*, 27833–27842. DOI: dx.doi.org/10.1021/jp506637v
37. Lazaridis, F.; **Savara, A.**; Argyrakis, P. “Reaction efficiency effects on binary chemical reactions” *J. Chem. Phys.*, **2014**, *141*, 104103.
DOI: 10.1063/1.4894791

38. **Savara, A.** “Vibrational spectra of CO adsorbed on oxide thin films: A tool to probe the surface defects and phase changes of oxide thin films” *J. Vac. Sci Technol. A*, **2014**, *32*, 021505. doi: 10.1116/1.4858619
39. **Savara, A.**; and Weitz, E.; “Elucidation of Intermediates and Mechanisms in Heterogeneous Catalysis Using Infrared Spectroscopy” *Ann. Rev. Phys. Chem.*, **2014**, *65*, 249-273.
**Invited Review
40. **Savara, A.** “Standard States for Adsorption on Solid Surfaces: 2D Gases, Surface Liquids, and Langmuir Adsorbates” *J. Phys. Chem. C*, **2013**, *117*, 15710–15715.
41. **Savara, A.**; Ludwig, W.; Dostert, K.-H.; Schauer mann, S. “Temperature dependence of the 2-butene hydrogenation over supported Pd nanoparticles and Pd(111)” *J. Mol. Catal.* **2013**, *377*, 137-142.
42. **Savara, A.**; Ludwig, W.; Madix, R.J.; Schauer mann, S.; and Freund, H.-J. “Kinetic Evidence for a Non-Langmuir-Hinshelwood Surface Reaction: H/D Exchange over Pd Nanoparticles and Pd(111).” *ChemPhysChem*, **2013**, *14*, 1686-1695. DOI: 10.1002/cphc.201300179
**Editor’s Choice
43. Liu, W.; **Savara, A.**; Ren., X.; Ludwig, W.; Dostert, K.-H.; Schauer mann, S.; Tkatchenko, A.; Freund, H.-J.; and Scheffler, M. “Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111)” *J. Phys. Chem. Lett.* **2012**, *3*, 582–586.
44. Ludwig, W.; **Savara, A.**; Madix, R.J.; Schauer mann, S.; and Freund, H.-J. “Subsurface Hydrogen Diffusion into Pd Nanoparticles: Role of Low-Coordinated Sites and Facilitation by Carbon” *J. Phys. Chem. C*, **2012**, *116*, 3539–3544
45. Ludwig, W.; **Savara, A.**; Dostert, K.-H.; Schauer mann, S. “Olefin hydrogenation on Pd model supported catalysts: New mechanistic insights.” *J. Catal*, **2011**, *284*, 148-156.
46. Ludwig, W.; **Savara, A.**; Brandt, B.; and Schauer mann, S. “A Kinetic Study on the Conversion of *Cis*-2-butene with Deuterium on a Pd/Fe₃O₄ Model Catalyst.” *Phys. Chem. Chem. Phys.*, **2011**, *13*, 966-977.
47. **Savara, A.**; and Weitz, E. “Kinetics of $\text{NO} + \text{H}^+ + \text{NO}_3^- \rightarrow \text{NO}_2 + \text{HNO}_2$ on BaNa-Y: Evidence for a Diffusion-Limited $\text{A} + \text{B} \rightarrow 0$ Reaction on a Surface.” *J. Phys. Chem.*, **2010**, *114*, 20621–20628.
48. Ludwig, W.; **Savara, A.**; Schauer mann, S.; and Freund, H.-J. “Role of Low-Coordinated Surface Sites in Olefin Hydrogenation: A Molecular Beam Study on Pd Nanoparticles and Pd(111).” *ChemPhysChem*, **2010**, *11*, 2319 – 2322.

49. Ludwig, W.; **Savara, A.**; and Schauer mann, S. "Role of Hydrogen in Olefin Isomerization and Hydrogenation: A Molecular Beam Study on Pd Model Supported Catalysts." *Dalton Trans.*, **2010**, 39, 8484–8491.
50. **Savara, A.**; Sachtler, W.M.H.; and Weitz, E. "TPD of NO₂⁻ and NO₃⁻ from Na-Y: The Relative Stabilities of Nitrates and Nitrites in Low Temperature DeNO_x Catalysis." *Appl. Catal. B*, **2009**, 90, 120-125.
51. **Savara, A.**; Danon, A; Sachtler, W.M.H.; and Weitz, E. "TPD of Nitric Acid on BaNa-Y: Evidence that a Nanoscale Environment Can Alter a Reaction Mechanism." *Phys. Chem. Chem. Phys*, **2009**, 11, 1180-1188.
52. **Savara, A.**; Schmidt, C.; Geiger, F.M.; and Weitz, E. "Adsorption Entropies and Enthalpies and Their Implications for Adsorbate Dynamics." *J. Phys. Chem. C*, **2009**, 113, 2806-2815.
53. Yeom, Y.; Li, M.; **Savara, A.**; Sachtler, W.M.H.; and Weitz, E. "Mechanisms of NO_x Reduction with Oxygenates Over Zeolite and γ -Al₂O₃ Catalysts." *Catalysis Today*, **2008**, 136, 55-63.
54. **Savara, A.**; Li, M.; Sachtler, W.M.H.; and Weitz, E. "Catalytic Reduction of NH₄NO₃ by NO: Effects of Solid Acids and Implications for Low Temperature DeNO_x Processes." *Appl. Catal. B* **2008**, 81, 251-257.
55. Schmidt, C.; **Savara, A.**; Weitz, E.; and Geiger, F.M. "Enthalpy and Entropy of Acetone Interacting with Degussa P25 TiO₂ Determined by Chemical Ionization Mass Spectrometry." *J. Phys. Chem. C* **2007**, 111, 8260-8267.

B) Books and Theses

1. **Savara, A.**; *Kinetic, Thermodynamic, and Mechanistic Studies of DeNO_x Catalysis over BaNa-Y: The Roles of Nitrates and Nitrites*. Northwestern University, Evanston, IL, **2008**.

C) Organizing of Conferences, Symposia, and Workshops

1. "Open-Source Software in Chemistry" Workshop Event Director. ACS Fall 2022 National Meeting, Chicago, IL, August 2022.
2. "PEUQSE: Bayesian Parameter Estimation for Comparing Observations and Predictions" Workshop. ACS Fall 2022 National Meeting, Chicago, IL, August 2022.
3. "MSRESOLVE: Quantitative Extractions of Concentrations from Mass Spectrometry Without Reference Patterns" Workshop. ACS Fall 2022 National Meeting, Chicago, IL, August 2022.
4. "KMCOS : Introduction to Kinetic Monte Carlo of Systems" Workshop. ACS Fall 2022 National Meeting, Chicago, IL, August 2022.

5. "Open-Source Software for Kinetics, Chemical Networks, & Reactor Modeling" Division: CATL. ACS Fall 2022 National Meeting, Chicago, IL. August, 2022.
6. "Bridging Surface Science to Catalysis" Division: CATL. ACS Spring 2022 National Meeting, San Diego, CA. March, 2022.
7. Co-Director for #ChemistsLive cross divisional virtual event across CATL and BIOL, September, 2020. (*Virtual. >80 speakers, >400 attendees.*)
8. "Scale up and Multi-Scale Modeling" Division: CATL. ACS Fall 2020 National Meeting, San Francisco, CA, August, 2020. (*Virtual*)
9. "Catalysis for Environmental and Energy Applications" Division: CATL. ACS Spring 2020 National Meeting, Philadelphia, PA. March, 2020. (*Virtual*)
10. Program Chair for ACS Division of Catalysis (CATL) for 257th ACS National Meeting, Orlando, FL. March 31-April 04, 2019.
11. "Catalysis for Environmental and Energy Applications" Division: ENVR & CATL. 258th ACS National Meeting, San Diego, CA. August 25-29, 2019.
12. "Advances in Methods for Comparing Molecular & Supramolecular Simulations to Experiments" Division: CATL & PHYS & COMP & CINF. 257th ACS National Meeting, Orlando, FL. March 31- April 04, 2019.
13. "Elucidation of Mechanisms & Kinetics on Surfaces" Division: CATL & PHYS & INOR & ENFL & ENVR. 257th ACS National Meeting, Orlando, FL. March 31- April 04, 2019.
14. "ACS Award in Surface Chemistry: Symposium in Honor of Hajo Freund" Division: COLL & CATL & PHYS. 257th ACS National Meeting, Orlando, FL. March 31- April 04, 2019.
15. "Catalysis for Environmental and Energy Applications" Division: ENVR & CATL. 256th ACS National Meeting, Boston, MA. August 19-23, 2018.
16. Program Chair for ACS Division of Catalysis (CATL) for 255th ACS National Meeting, New Orleans, LA. March 18-22, 2018.
17. "Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts" Division: CATL & ENFL & COMP. 255th ACS National Meeting, New Orleans, LA. March 18-22 2018.
18. "Elucidation of Mechanisms & Kinetics on Surfaces" Division: CATL & ENVR. 255th ACS National Meeting, New Orleans, LA. March 18-22 2018.
19. "Heterogeneous Catalysis for Environmental and Energy Applications" Division: ENVR & CATL. 254th ACS National Meeting, Washington, DC. August 20-24, 2017.
20. Program Chair for ACS Division of Catalysis (CATL) for 237th ACS National Meeting, San Francisco, CA. Apr 2-6, 2017.
21. "Elucidation of Mechanisms & Kinetics on Surfaces" Division: COLL & ENVR & CATL. 253rd ACS National Meeting, San Francisco, CA. Apr 2-6, 2017.
22. "Applied Catalysis for Environmental Applications" Division: ENVR & CATL. 252nd ACS National Meeting, San Diego, CA. August 21-25, 2016.
23. "Elucidation of Mechanisms & Kinetics on Surfaces" Division: CATL, COLL, PHYS. 251st ACS National Meeting. San Diego, California. March 13-17, 2016.
24. "Heterogeneous Catalysis for Environmental and Energy Applications" Division: ENVR & CATL. 250th ACS National Meeting, Boston, MA. August 16-17, 2015.
25. "Elucidation of Mechanisms & Kinetics on Surfaces" Division: COLL. 249th ACS National Meeting. Denver, Colorado. March 22-26, 2015.
26. "Heterogeneous Catalysis for Environmental and Energy Applications" ENVR, CATL at 248th ACS National Meeting in San Francisco (August 13th-14th, 2014).
27. "Catalysis Science: The Next Generation" Division: CATL. 247th ACS National Meeting, Dallas, TX. March 16, 2014.

D) Invited Presentations

1. Chen, B.; Xu, Y.; Xiong, C.; Rickard, S.; Boscoboinik, J.; Jiang, D.-e.; Kidder, M.; **Savara, A.**, “Conversion of Ethanol over LaSrMnO₃ catalysts: Mechanistic Insights from Single Crystals to Powders on the Roles of Oxygen Vacancies.” ACS Spring 2022 National Meeting, **2022**.
2. **Savara, A.**; Walker, E.A.; “Bayesian Parameter Estimation (BPE) as a method for Connecting Theory to Experiment.” ACS Spring 2022 National Meeting, **2022**.
3. **Savara, A.**; Matera, S.; “Kinetic Monte Carlo of Systems (KMCOS). Connecting Electronic Structure Calculations to Experiment by Simulations, an Update.” ACS Fall 2021 National Meeting & Expo. Virtual. **2021**.
4. **Savara, A.**; Walker, E.A.; “Harnessing data sets for more accurate kinetic parameter estimation: Bayesian parameter estimation to include errors from both experiment and theory.” ACS Spring 2020 National Meeting & Expo. Virtual. **2020**.
<https://doi.org/10.1021/scimeetings.0c00082> Also presented by invitation during the @CAT symposium on March 28th 2020.
5. Sutton, J.; Lorenzi, J.; Krogel, J.; Xiong, Q.; Pannala, S.; Matera, S.; **Savara, A.**, Multiscale Modeling, Coupling Dft to KMC to CFD and Comparison to Experiment: A Success Story with CO Oxidation over RuO₂. In Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2019**; Vol. 257.
6. Danielson, T.; Sutton, J.; Hin, C.; **Savara, A.**, Sqertss & Sqertt: Dynamic Throttling of KMC Rate Constants to Achieve Experimental Timescales in Simulations. In Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2019**; Vol. 257.
7. **Savara, A.**; Sawtelle, S., Kinetic Simulations and Parameter Estimation: Bayesian Kinetic Parameter Estimation to Include Errors from Both Experiment and Theory. In Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2019**; Vol. 257.
8. Sutton, J.; Danielson, T.; Beste, A.; **Savara, A.**, Low Temperature C-H Bond Breaking on an Inexpensive Metal Oxide: Methanol to Formaldehyde on Cerium Oxide. In Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2018**; Vol. 256.
9. **Savara, A.**; Sutton; Danielson; Hin; Lorenzi; Matera; Kinetic Simulations of Catalysis: From Multiple Surfaces to Physical Mixtures. International Conference on Theoretical Aspects of Catalysis, UCLA campus, Los Angeles, California, USA. June 24, **2018**.
10. Sutton, J.; Lorenzi, J.; Matera, S.; **Savara, A.**, Multiscale Modeling from Electrons to Reactors: CO Oxidation over RuO₂. In Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2018**; Vol. 255.
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15. **Savara, A.**; Elucidation of Kinetics and Mechanisms on Surfaces: From Ultrahigh Vacuum Environments to Liquid Phase Environments. University of Cincinnati, Cincinnati, OH, Dec 18, **2017**.
16. **Savara, A.**; Campbell, C., Standard States of Adsorbates on Surfaces. In *Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: 2017*; Vol. 253.
17. **Savara, A.**; Chan-Thaw, C.; Rossetti, I.; Prati, L.; Villa, A., Collision Theory in Liquids and the Molecular Origin of the Selectivity Difference between AuPd and Pd for Benzylic Alcohol Oxidation. In *Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: 2017*; Vol. 253.
18. **Savara, A.**, Simulation of Temperature Programmed Reactions: Tpr Mechanism Following Adsorption of Methanol on CeO₂ (111). In *Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: 2016*; Vol. 251.
19. **Savara, A.**; Simulation of Temperature Programmed Reactions: TPR Mechanism Following Adsorption of Methanol on CeO₂(111), Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany June 3, **2016**.
20. **Savara, A.**; Elucidation of Kinetics and Mechanisms on Surfaces: From Ultrahigh Vacuum Environments to Liquid Phase Environments. University of Central Florida, Orlando, FL 32816, April 21, **2016**.
21. **Savara A.**; Elucidation of Kinetics and Mechanisms on Surfaces: From Ultrahigh Vacuum Environments to Liquid Phase Environments. New Mexico State University, 1175 North Horseshoe Dr., Las Cruces, NM 88003, Feb 25, **2016**.
22. **Savara A.**; Kinetic Simulations of Reactions on Surfaces: From Equations to Probabilistic Models. Kennesaw State University, 370 Paulding Avenue NW, MD#1203, Kennesaw, GA 30144, Feb 2, **2016**.
23. **Savara, A.**; Chan-Thaw, C.; Rossetti, I.; Villa, A.; Prati, L., Mechanism for Benzyl Alcohol Oxidation on Carbon-Supported Pd Nanoparticles. In *Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: 2015*; Vol. 250.
24. **Savara, A.**; Kandziolka, M.; Kidder, M.; Gill, L.; Wu, Z., Aromatic-Hydroxyl Interaction of a Lignin Model-Compound on Sba-15, Present at Pyrolysis Temperatures. In *Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: 2015*; Vol. 250.
25. **Savara, A.**; Endothermic Spillover of Adsorbates and Organic Oxygenate Interactions with Metal Oxide Surfaces. University of Tennessee, Knoxville. Estabrook Road, Knoxville TN. November 29, **2013**.
26. **Savara, A.**; The roles of subsurface hydrogen in hydrogenation over Pd surfaces, and in H/D exchange over Pd surfaces. Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, TN 37931, July 20, **2011**.
27. **Savara, A.**; The roles of subsurface hydrogen in hydrogenation over Pd surfaces, and in H/D exchange over Pd surfaces, and Acid Catalyzed Reduction of NH₄NO₃ by NO and its Role in Low T DeNO_x Catalysis. BASF Corporation, 25 Middlesex-Essex Turnpike, Iselin NJ 08830, June 14, **2011**.
28. **Savara, A.**; The roles of subsurface hydrogen in hydrogenation over Pd surfaces, and in H/D exchange over Pd surfaces. UOP/Honeywell Specialty Materials, Technology R&D, 25 E. Algonquin Rd., Des Plaines, IL 60017. June 10, **2011**.

29. **Savara, A.**; The roles of subsurface hydrogen in hydrogenation over Pd surfaces, and in H/D exchange over Pd surfaces. University of Delaware, 210 S College Ave, Newark, DE 19716, Jan 24, **2011**.

E) Conferences Presented At (Conference List Only)

- 2022 American Chemical Society Spring National Meeting (ACS)
- 2021 American Chemical Society Fall National Meeting (ACS)
- 2021 18th International Conference on Theoretical Aspects of Catalysis (ICTAC)
- 2020 American Chemical Society Fall National Meeting (ACS)
- 2020 American Chemical Society Spring National Meeting
- 2019 18th Southeastern Catalysis Society Meeting (SECS)
- 2019 257th National American Chemical Society Meeting (ACS)
- 2018 256th National American Chemical Society Meeting (ACS)
- 2018 17th International Conference on Theoretical Aspects of Catalysis (ICTAC)
- 2018 255th National American Chemical Society Meeting (ACS)
- 2017 16th Southeastern Catalysis Society Meeting (SECS)
- 2017 254th National American Chemical Society Meeting (ACS)
- 2017 253rd National American Chemical Society Meeting (ACS)
- 2016 15th Southeastern Catalysis Society Meeting (SECS)
- 2016 251st National American Chemical Society Meeting (ACS)
- 2015 14th Southeastern Catalysis Society Meeting (SECS)
- 2015 250th American Chemical Society National Meeting (ACS)
- 2014 13th Southeastern Catalysis Society Meeting (SECS)
- 2015 249th American Chemical Society National Meeting (ACS)
- 2013 246th American Chemical Society National Meeting (ACS)
- 2013 23rd North American Catalysis Society Meeting (NAM)
- 2012 244th American Chemical Society National Meeting (ACS)
- 2010 57th American Vacuum Society Meeting (AVS)
- 2010 Gordon Research Conference on Catalysis (GRC)
- 2009 26th European Conference on Surface Science (ECOSS)
- 2007 20th North American Catalysis Society Meeting (NAM)
- 2007 233rd American Chemical Society National Meeting (ACS)
- 2006 231st American Chemical Society National Meeting (ACS)
- 2003 225th American Chemical Society National Meeting (ACS)

F) Reviewer for

Journal of the American Chemical Society, RSC Advances, ACS Catalysis, Journal of Catalysis, Topics in Catalysis, Catalysis Letters, Journal of Physical Chemistry, Physical Chemistry Chemical Physics, Applied Catalysis A, Applied Catalysis B, AIChE Journal, Surface Science, ChemSusChem, Catalysis Science and Technology, Chemical Engineering Research and Design, Applied Materials and Interfaces, Journal of Physics and Chemistry of Solids, Catalysts, Chemical Engineering Science, Chemical Papers, Materials Research Society Spring Meeting, International Journal of Hydrogen Energy, Department of Energy Basic Energy Sciences, American Chemical Society Petroleum Research Fund.

G) Collaborators (Past 48 months and Selected Close Collaborators):

- Florencia C. Calaza, Fritz-Haber-Institut der Max-Planck-Gesellschaft
- Carine Chan-Thaw, Dept of Chimica Inorganica Metallorganica e Analitica, University of Milan
- Karl-Heinz Dostert, Fritz-Haber-Institut der Max-Planck-Gesellschaft
- Hans-Joachim (“Hajo”) Freund, Fritz-Haber-Institute of the Max Planck Society
- Rachel Getman, Clemson University
- Celine Hin, Virginia Tech
- Cong Liu, Argonne National Lab
- Wei Liu, Fritz-Haber-Institut der Max-Planck-Gesellschaft
- Wiebke Ludwig, Fritz-Haber-Institute of the Max Planck Society
- Sebastian Matera, Freie Universität, Berlin
- Juan Lorenzi, Technischen Universität, Munich
- Steve Overbury, Oak Ridge National Laboratory
- Laura Prati, Department of Chimica Inorganica Metallorganica e Analitica, University of Milan
- Ilenia Rossetti, Department of Chimica Inorganica Metallorganica e Analitica, University of Milan
- Svetlana Schauerermann, Fritz-Haber-Institute of the Max Planck Society
- Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft
- Alexandre Tkatchenko, Fritz-Haber-Institut der Max-Planck-Gesellschaft
- Alberto Villa, Department of Chimica Inorganica Metallorganica e Analitica, University of Milan
- Ye Xu, Louisiana State University, Baton Rouge

H) Students and Postdocs Mentored:

- 2012 & 2013 Zachary Coin (Undergraduate Student) ORNL / UTK
- 2012 & 2013 Michael Kandziolka (Undergraduate Student) ORNL / UTK
- 2013 Subeer Talapatra (Undergraduate Student) ORNL / UVA
- 2013 Anna Wanhala (Undergraduate Student) ORNL / Albion College
- 2014 William Hawks (Undergraduate Student) ORNL / UTK
- 2014 Christa Cody (Undergraduate Student) ORNL / Tennessee Tech
- 2014 & 2015 Thomas Danielson (Graduate Student) ORNL / Virginia Tech
- 2015 Stacie Schroll (Undergraduate Student) ORNL / Kellogg Community College
- 2015 Christopher Elliott (Undergraduate Student) ORNL / Covenant College
- 2016 Elizabeth E. Bickel (Undergraduate Student) ORNL / Tennessee Tech
- 2016 Wilson Jeter (Undergraduate Student) ORNL / Tulane
- 2016 & 2017 Chris Nellis (Graduate Student) ORNL / Virginia Tech
- 2016 & 2017 Yafen Zhang (Postdoctoral Researcher) ORNL
- 2016 & 2017 Jonathan Sutton (Postdoctoral Researcher) ORNL
- 2017 Erick Holguin (Undergraduate Student) ORNL / UNC Greensboro
- 2017 Sean Hentschel (Undergraduate Student) ORNL / Miami Dade College
- 2017 Hung Vuong (Undergraduate Student) ORNL / Grinnell College
- 2017 & 2018 Charles Watt (Undergraduate Student) ORNL / Princeton
- 2018 Alexander Rogers (Undergraduate Student) ORNL / University of TN – Knoxville
- 2018 Andrea Kraetz (Undergraduate Student) ORNL / Arizona State University
- 2018 Kaitlyn Lawrence (Undergraduate Student) ORNL / Auburn University
- 2018 & 2019 Bo Chen (Postdoctoral Researcher) ORNL
- 2019 Caspar Lant (Undergraduate Student) ORNL / New York University
- 2019 Shane Rickard (Undergraduate Student) ORNL / St. John Fisher College
- 2020 Tyler Pleasant (Post Undergraduate Student) ORNL / MIT

- 2020 Christopher Hayes (Undergraduate Student) ORNL / Stonybrook
- 2020 & 2021 Shalini Jayaraman Rukmani (Postdoctoral Researcher) ORNL
- 2021 Russell Burgett (Undergraduate Student) ORNL / Iowa State University
- 2021 & 2022 Lane Lee (Undergraduate Student) ORNL / Roane State Community College
- 2022 Meelod Waheed (Undergraduate Student) ORNL / Northern Virginia Community College
- 2022 Troy Gustke (Undergraduate Student) ORNL / Virginia Tech

I) Leadership and Service Positions

- 2018-2022 ACS Catalysis Division Councilor
- 2021-2022 ACS Division Activities Committee (*National*)
- 2020 ACS Meetings and Expositions Committee (*National*)
- 2020-2022 ACS Multidisciplinary Program Planning Group (*National*)
Member-At Large
- 2017-2022 ACS Multidisciplinary Program Planning Group (*National*)
CATL Division Representative
- 2017-2019 ACS Catalysis Division Spring Program Chair
- 2016-2019 ACS Environmental Division Membership Chair
- 2012-2015 ACS Environmental Division Secretary
- 2012-Present ACS Environmental Division Webmaster
- 2012-2018 Southeastern Catalysis Society Webmaster
- 2004-2008 Northwestern University Graduate Leadership Council
- 2006-2007 Northwestern University Graduate Student Association President
- 2004-2006 Northwestern University Graduate Student Association VP

J) Journal Articles Acknowledging A. Savara

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