CURRICULUM VITAE

NAME: ADITYA (ASHI) SAVARA **CITIZENSHIP:** US

AFFILIATIONS: STAFF SCIENTIST, OAK RIDGE NATIONAL LAB
ADJUNCT PROFESSOR, VIRGINIA TECH (MAT. SCI. & ENG.)
PROFESSIONAL ORGANIZATIONS: ACS, NACS, AVS, IUPAC

PROFILE

Heterogeneous catalysis, chemical kinetics, complex reaction mechanisms, chemistry of surfaces: adsorption, diffusion, 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**

- Kinetic Monte Carlo algorithmic enhancements to enable molecular level investigations of chemical kinetics as well as reactor scale simulations based on molecular modeling (SQERTSS, ppSSD).
- Elucidation of the kinetics and mechanism in benyzlic alcohol oxidation over Pd and AuPd nanoparticles for greener alcohol oxidation. *(2 Journal Covers)*
- Kinetic simulations of complex reaction networks (CRNs) and organic oxygenates on oxides, including acid-base bifunctional catalysis for aldol condensation
- Kinetic Monte Carlo simulations of endothermic spillover and entropy implications.
- Construction of a molecular beam apparatus for experimental measurement of the chemical kinetics of surface reactions and catalyt processes.
- Infrared discovery of aromatic-hydroxyl interactions for BPEa-SBA-15, a lignin model compound, with the interaction present at pyrolysis temperatures. *(1 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 $H_2/D_2/HD$. *(Featured as Editors Choice)*

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

- Reaction kinetics of NOx reduction over Ba-Y zeolites and related catalysts.
- First observation that nanoscale pores can alter a reaction mechanism.
- Discovered the acid catalyzed reduction of NH_4NO_3 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.

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OAK RIDGE NATIONAL LABORATORY , CHEMICAL SCIENCES DIVISION

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

- 2007 ACS Graduate Student Award in Environmental Chemistry
- 2004 Keynote Speaker for NU New Teaching Assistants Luncheon
- 2004 NU WCAS Outstanding Graduate Student Teacher Award University-wide
- 2004 PLU L. Carroll King Award for Excellence in 100-Level Teaching (Department)
- 2003 University of Hawaii's Dean's List
- 2000 Hawaii Representative in National Chemistry Olympiad

LEADERSHIP & SERVICE

- 2017-2019 ACS MPPG Committee
- 2018-2019 ACS CATL Division Councilor
- 2017-2019 ACS Catalysis Division Spring Program Chair
- 2016-2019 ACS Environmental Division Membership Chair
- 2012-2015 ACS Environmental Division Secretary
- 2006-2007 NU Graduate Student Association President
- 2004-2006 NU 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. **2017-2019 $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 CNMS Proposal ID: CNMS2014-306 Reducible Versus Irreducible Transition Metal Cation Activation of Carbonyl Compounds for Nucleophilic Attack Mechanisms Such As Aldol Condensation. **2014-2015. Two weeks of computational effort.** PI.
- ORNL DOE LDRD project ID: 7427 Predictive computational catalysis: From electrons to reactors. **2015-2017 $1,159,000.** PI.
- ORNL CSD PD project ID: 7550 Hydrogen production membrane reactor. **2013-2014. $12,000.** 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.

Publication List of Aditya Savara

45+ Journal Articles, h-index of 15

A) Journal Articles

1. **Savara, A.* "**Microkinetic Simulation and Fitting of the Temperature Programmed Reaction of Methanol on CeO_2(111): H_2 and H_2O + V Production." *React. Kinet. Mech. Cat.*, **2020**, *Accepted.*

2. Matera, S.; Schnieder, 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**

3. 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**

4. Zhang, Y.; Mullins, D.R.; **Savara, A.*** "Effect of Sr Substitution in $LaMnO_3$(100) on Catalytic Conversion of Acetic Acid to Ketene and Combustion-like Products" *J. Phys Chem. C.* **2019,** *123*, 4148-4157.

5. 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**

6. Chan-Thaw CE, **Savara A,** Villa A.; Selective Benzyl Alcohol Oxidation over Pd Catalysts. *Catalysts*, **2018**, *8*, 431.
   ****Invited Review**

7. 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.

8. 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.

9. **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**

10. 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.

11. 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 RuO_2" *ACS Catalysis **2018**, 8, 5002-5016.*

12. 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

13. 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 CeO_2(111)" *J. Phys. Chem. Lett.*, **2017**, *8*, 5810–5814. DOI: 10.1021/acs.jpclett.7b02683
    **** ACS Liveslides:** https://pubs.acs.org/doi/suppl/10.1021/acs.jpclett.7b02683

14. 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.

15. W. Liu; Y. Jiang; K.-H. Dostert; C. P. O'Brien; W. Riedel; **A. Savara**; S. Schauermann and A. Tkatchenko; "Catalysis beyond frontier molecular orbitals: Selectivity in partial hydrogenation of multi-unsaturated hydrocarbons on metal catalysts." *Sci. Adv.* **2017**. DOI: 10.1126/sciadv.1700939

16. **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

17. 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

18. **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)

19. **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

20. 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

21. **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

22. **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**

23. K.-H. Dostert; C. P. O'Brien; W. Liu; W. Riedel; **A. Savara**; A. Tkatchenko; S. Schauermann and H.-J. Freund. "Adsorption of isophorone and trimethyl-cyclohexanone 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

24. 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.

25. **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

26. 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**

27. Dostert, K.-H.; O'Brien, C.P.; Ridel, W.; **Savara, A.**; Liu, W.; Oehzelt, M.; Tkatchenko, A.; Schauermann, 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

28. Lazaridis, F.; **Savara, A.**; Argyrakis, P. "Reaction efficiency effects on binary chemical reactions" *J. Chem. Phys.*, **2014**, *141*, 104103. DOI: 10.1063/1.4894791

29. **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

30. **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**

31. **Savara, A.** "Standard States for Adsorption on Solid Surfaces: 2D Gases, Surface Liquids, and Langmuir Adsorbates" *J. Phys. Chem. C*, **2013**, *117*, 15710–15715.

32. **Savara, A.**; Ludwig, W.; Dostert, K-H.; Schauermann, S. "Temperature dependence of the 2-butene hydrogenation over supported Pd nanoparticles and Pd(111)" *J. Mol. Catal.* **2013,** *377*, 137-142.

33. **Savara, A.**; Ludwig, W.; Madix, R.J.; Schauermann, 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**

34. Liu, W.; **Savara, A.**; Ren., X.; Ludwig, W.; Dostert, K.-H.; Schauermann, 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**.**

35. Ludwig, W.; **Savara, A.**; Madix, R.J.; Schauermann, 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

36. Ludwig, W.; **Savara, A.**; Dostert, K.-H.; Schauermann, S. "Olefin hydrogenation on Pd model supported catalysts: New mechanistic insights." *J. Catal*, **2011**, *284*, 148-156.

37. Ludwig, W.; **Savara, A.**; Brandt, B.; and Schauermann, S. "A Kinetic Study on the Conversion of *Cis*-2-butene with Deuterium on a Pd/Fe_3O_4 Model Catalyst." *Phys. Chem. Chem. Phys.*, **2011**, *13*, 966-977.

38. **Savara, A.**; and Weitz, E. "Kinetics of $NO + H^+ + NO_3^- \rightarrow NO_2 + HNO_2$ on BaNa-Y: Evidence for a Diffusion-Limited $A + B \rightarrow 0$ Reaction on a Surface." *J. Phys. Chem.*, **2010**, *114*, 20621–20628.

39. Ludwig, W.; **Savara, A.**; Schauermann, 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.

40. Ludwig, W.; **Savara, A.**; and Schauermann, S. "Role of Hydrogen in Olefin Isomerization and Hydrogenation: A Molecular Beam Study on Pd Model Supported Catalysts." *Dalton Trans.*, **2010**, *39*, 8484–8491.

41. **Savara, A.**; Sachtler, W.M.H.; and Weitz, E. "TPD of NO_2^- and NO_3^- from Na-Y: The Relative Stabilities of Nitrates and Nitrites in Low Temperature DeNOx Catalysis." *Appl. Catal. B*, **2009**, *90*, 120-125.

42. **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.

43. **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.

44. Yeom, Y.; Li, M.; **Savara, A.**; Sachtler, W.M.H.; and Weitz, E. "Mechanisms of NOx Reduction with Oxygenates Over Zeolite and γ-Al_2O_3 Catalysts." *Catalysis Today*, **2008**, *136*, 55-63.

45. **Savara, A.**; Li, M.; Sachtler, W.M.H.; and Weitz, E. "Catalytic Reduction of NH_4NO_3 by NO: Effects of Solid Acids and Implications for Low Temperature DeNOx Processes." *Appl. Catal. B* **2008**, *81*, 251-257.

46. Schmidt, C.; **Savara, A.**; Weitz, E.; and Geiger, F.M. "Enthalpy and Entropy of Acetone Interacting with Degussa P25 TiO_2 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 DeNOx Catalysis over BaNa-Y: The Roles of Nitrates and Nitrites.* Northwestern University, Evanston, IL, **2008**.

C) Conferences & Symposia Organized

1. "Catalysis for Environmental and Energy Applications" Division: ENVR & CATL. 258th ACS National Meeting, San Diego, CA. August 25-29, 2019.
2. Program Chair for ACS Division of Catalysis (CATL) for 257th ACS National Meeting, Orlando, FL. March 31- April 04, 2019.
3. "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.

4. “Elucidation of Mechanisms & Kinetics on Surfaces” Division: CATL & PHYS & INOR & ENFL & ENVR. 257th ACS National Meeting, Orlando, FL. March 31- April 04, 2019.
5. “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.
6. “Catalysis for Environmental and Energy Applications” Division: ENVR & CATL. 256th ACS National Meeting, Boston, MA. August 19-23, 2018.
7. Program Chair for ACS Division of Catalysis (CATL) for 255th ACS National Meeting, New Orleans, LA. March 18-22, 2018.
8. “Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts” Division: CATL & ENFL & COMP. 255th ACS National Meeting, New Orleans, LA. March 18-22 2018.
9. “Elucidation of Mechanisms & Kinetics on Surfaces” Division: CATL & ENVR. 255th ACS National Meeting, New Orleans, LA. March 18-22 2018.
10. “Heterogeneous Catalysis for Environmental and Energy Applications” Division: ENVR & CATL. 254th ACS National Meeting, Washington, DC. August 20-24, 2017.
11. Program Chair for ACS Division of Catalysis (CATL) for 237th ACS National Meeting, San Francisco, CA. Apr 2-6, 2017.
12. “Elucidation of Mechanisms & Kinetics on Surfaces” Division: COLL & ENVR & CATL. 253rd ACS National Meeting, San Francisco, CA. Apr 2-6, 2017.
13. “Applied Catalysis for Environmental Applications” Division: ENVR & CATL. 252nd ACS National Meeting, San Diego, CA. August 21-25, 2016.
14. “Elucidation of Mechanisms & Kinetics on Surfaces” Division: CATL, COLL, PHYS. 251sth ACS National Meeting. San Diego, California. March 13-17, 2016.
15. “Heterogeneous Catalysis for Environmental and Energy Applications” Division: ENVR & CATL. 250th ACS National Meeting, Boston, MA. August 16-17, 2015.
16. “Elucidation of Mechanisms & Kinetics on Surfaces” Division: COLL. 249th ACS National Meeting. Denver, Colorado. March 22-26, 2015.
17. "Heterogeneous Catalysis for Environmental and Energy Applications" ENVR,CATL at 248th ACS National Meeting in San Francisco (August 13th-14th, 2014).
18. “Catalysis Science: The Next Generation” Division: CATL. 247th ACS National Meeting, Dallas, TX. March 16, 2014.

D) Invited Presentations

1. 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.
2. 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.
3. **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.
4. Sutton, J.; Danielson, T.; Beste, A.; **Savara, A.**, Low Temperature Ch 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.

5. **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**.
6. 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.
7. Vuong, H.; Binder, A.; Sutton, J.; **Savara, A.** In Experimental Data Based Combinatorial Kinetic Simulations for Predictions of Enhanced Exhaust Emission Catalysis with Bifunctional Mixed-Bed Systems, Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2018**.
8. Zhang, Y.; Garzon, F. P.; Kidder, M.; Mullins, D.; **Savara, A.,** Conversion of Alcohols over Lamno3 and La0. 7sr0. 3mno3 in the Presence and Absence of Oxygen. In Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2018**; Vol. 255.
9. **Savara, A.;** Elucidation of Kinetics and Mechanisms on Surfaces: From Ultrahigh Vacuum Environments to Liquid Phase Environments. Virginia Tech, Blacksburg, Virginia, Jan 29, **2018**.
10. **Savara, A.**, Microkinetic Modeling and Molecular Origin of the Selectivity Differences between Palladium and Gold-Palladium in Benzyl Alcohol Oxidation. In Abstr Pap Am Chem S, Amer Chemical Soc 1155 16th ST, Northwest, Washington, DC 20036 USA: **2017**; Vol. 254.
11. **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**.
12. **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.
13. **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.
14. **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.
15. **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.**
16. **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**.
17. **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**.
18. **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.**
19. **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.

20. **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.
21. **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**.
22. **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.**
23. **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 DeNOx Catalysis. BASF Corporation, 25 Middlesex-Essex Turnpike, Iselin NJ 08830, June 14, **2011.**
24. **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.**
25. **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)

- 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 Unversität, 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
- Swetlana Schauermann, 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: *

* Students with "ORNL" listed next to their name worked directly under my supervision at ORNL.

- 2010 Karl-Heinz Dostert (Graduate Student) Fritz Haber Institut, Germany
- 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

I) Leadership and Service Positions

- 2017-2019 ACS MPPG Committee
- 2018-2019 ACS CATL Division Councilor
- 2017-2019 ACS CATL Division Spring Program Chair
- 2016-2018 ACS ENVR Division Membership Chair
- 2012-2015 ACS ENVR Division Secretary
- 2014-2018 SECS Webmaster
- 2014-2018 SECS Webmaster
- 2004-2008 NU Graduate Leadership Council (4 Years)
- 2006-2007 NU Graduate Student Association President
- 2004-2006 NU Graduate Student Association VP