CONG LIU, Ph. D.

Argonne National Laboratory
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EDUCATION AND JOBS

Assistant Chemist, Argonne National Laboratory, 2016 – present
Argonne Director's Fellow, Argonne National Laboratory, 2013 – 2016
Ph. D., Physical Chemistry, University of North Texas, 2009 – 2013
1-year Graduate Training, Inorganic Chemistry, Shenyang University of Chemical Technology, China, 2007 – 2008
B. S., Applied Chemistry, Shenyang University of Chemical Technology, China, 2003 – 2007

RESEARCH

Assistant Chemist, Argonne National Laboratory (2016 – present)

- DOE BES Catalysis Program (co-PI), "Catalysis Science Program: Electronic Cooperativity in Supported Single- and Multinuclear-Sites for Catalytic C-C and C-H Bonds Functionalization", 2016 – present
- Research interests: Computational catalysts/materials design for energy conversion and storage, development of computational methods and models for complex catalytic systems, development of high-level quantum mechanical methods for solid-state catalysis

Argonne Director's Fellow, Argonne National Laboratory (2013 – 2016)

- Development of single-site metal catalysts for alkane functionalization
- Nanocatalyst design for catalytic and electrocatalytic CO_2 reduction and water splitting
- Computational studies of catalytic biomass conversion to fuels using zeolites
- Development of improved cathode materials for Li-ion batteries
- Development of composite nanomaterials for Li-air batteries
- Development of supported nanoparticles for fuel cell applications

Graduate Research Assistant, University of North Texas (2009 – 2013)
Research Advisor: Prof. Angela Wilson
Dissertation: "*Transition Metal Mediated C–O Bond Cleavage: From CO_2 Activation to Lignin Degradation*"

- CO_2 reactivity with homogeneous and heterogeneous transition metal catalysts
- Performance of density functional theory (DFT) methods on transition metal chemistry
- Computational studies of catalytic lignin degradation using transition metal complexes
- Computational drug design (Collaboration with Reata Pharmaceuticals, Inc)

Graduate Research Assistant, Shenyang University of Chemical Technology (2007 – 2008)
Research Advisor: Prof. Enjun Gao

- Synthesis of transition metal complexes with anti-cancer properties

Undergraduate Research Assistant, Shenyang University of Chemical Technology (2006 – 2007)

Thesis: "*Synthesis and Analysis of Rare Earth Element Containing LED Materials*"
- Synthesis and analysis of rear earth metal containing inorganic calcium LED compounds

FUNDINGS

- Co-PI: DOE BES Catalysis Program, "Catalysis Science Program: Electronic Cooperativity in Supported Single- and Multinuclear-Sites for Catalytic C-C and C-H Bonds Functionalization", $1.5M/yr, 2016 – present
- Co-PI: Argonne LDRD Program, "Data Science Enabled Catalyst Discovery", $100K, 2019
- Co-PI: U. Delaware-Argonne Seed Program, "Synergistic Multi-site Catalysis for Dry Reforming Processes", $70K/yr, 2018 – 2019
- PI: Argonne Director's Fellowship, $80K/yr, 2013 – 2016

HONORS

- Argonne Director's Fellow, Argonne National Laboratory, 2013 – 2016
- Chemical Computing Group (CCG) Research Excellence Award, 243th ACS National Meeting, 2012
- Outstanding International Graduate Student, University of North Texas, May 2013
- Thesis and Dissertation Fellowship, University of North Texas, 2012 – 2013
- Ed and Julia Hodges Memorial Scholarship for Outstanding Graduate Research, University of North Texas, June 2012
- Graduate Research Tuition Scholarship, University of North Texas, 2011 – 2012
- Poster Presentation Award, Southwest Theoretical Chemistry Conference, Oct. 2012
- First-place Presentation Award, 45th ACS Annual Meeting in Miniature DFW Section, April 2012
- Second-place Poster Presentation Award, Southwest Theoretical Chemistry Conference, Oct. 2010

LEADERSHIP AND SERVICE

- Review editor, Theoretical and Computational Chemistry Section, Frontiers in Chemistry, 2019 – present
- Review panel, Center for Functional Nanomaterials, Brookhaven National Laboratory, 2019 – present
- Reviewer, National Science Foundation (NSF) Chemistry Division, Chemical Theory, Models and Computational Methods program and Catalysis program, 2017 – present
- Session chair, Gordon Conference on Computational Chemistry, 2018
- Organizer, Computational Catalyst Design for Energy Conversion and Storage Symposium, 255th ACS National Meeting, 2018
- Volunteer presenter, Science Careers in Search of Women Conference, 2017 – 2018
- Abstract reviewer, North American Catalysis Society Meeting 2017
- Outstanding Reviewer, Computational and Theoretical Chemistry, 2015
- Session chair, COMP Program, 247th, 248th and 249th ACS National Meetings, 2014 – 2015
- Judge, Physical Chemistry Poster Award, 247th ACS National Meeting, 2014
- > 60 reviews for scientific journals including JACS, ACS Catalysis, Nano Energy, JPC, etc.

TEACHING AND MENTORING

Illinois Institute of Technology

- Guest lecture: "Computational Catalyst Design", Armour College of Engineering, March 2019

Argonne National Laboratory

- Postdocs: Prajay Patel (2019 – present), Dale Pahls (2017 – 2018), Meinan He (2017 – 2019, now at General Motors)
- Graduate students (DOE SCGSR Program): Colton Lund (UNT, 2020), Woochul Shin (OSU, 2019), J. Cesar Plascencia (MSU, 2017)
- Undergraduate students (DOE SULI Program): Nicholas Dewey (GVSU, 2019), Austin Pauga (NIU, 2018), Henry Dieckhaus (BC, 2018, Barry M. Goldwater award winner)

University of North Texas

- Teaching Assistant: CHEM 3452, Undergraduate Analytical Chemistry Lab, Spring 2009
- Graduate students, 2012 – 2013: Brandall Ingle (now postdoc at EPA), Michael Jones (now Pre-IRTA Fellow at NIH)
- Undergraduate student (REU Program, 2009 – 2010): Lloyd Munjanja (now scientist & director of Education, Outreach and Diversity, Emory U.)
- High school student (Texas TAMS Program, 2011 – 2013): Siva Manivasagam (Barry M. Goldwater award winner, now graduate student at U. Toronto)

Shenyang University of Chemical Technology

- Teaching Assistant: Undergraduate Physical Chemistry, Spring 2008
- Guest Lectures: Coordination Chemistry, Lecturer: Prof. E. Gao, Spring 2008

PUBLICATIONS

1. C. Byron, S. Bai, G. Celik, M. S. Ferrandon, **C. Liu**, C. Ni, A. Mehdad, M. Delferro, R. F. Lobo, A. V. Teplyakov. On the Role of Boron in Enhancing the Catalytic Performance of Supported Platinum Catalysts for Non-Oxidative Dehydrogenation of n-Butane. *ACS Catal.* **2020**, *10*(2), 1500.

2. W. Yao, Y. Yuan, G. Tan, **C. Liu**,***** M. Cheng, V. Yurkiv, X. Bi, F. Long, C. R. Friedrich, F. Mashayek, K. Amine, J. Lu, R. Tuning Li2O2 Formation Routes by Facet Engineering of MnO2 Cathode Catalysts. *J. Am. Chem. Soc.* **2019**, *141*(32), 12832.

3. D. M. Kaphan, M. S. Ferrandon, R. R. Langeslay, G. Celik, E. C. Wegener, **C. Liu**, J. Niklas, O. G. Poluektov, M. Delferro. Mechanistic Aspects of a Surface Organovanadium (III) Catalyst for Hydrocarbon Hydrogenation and Dehydrogenation. *ACS Catal.* **2019**, 9(12), 11055.

4. Y. A. Wu, I. McNulty, **C. Liu**, K. C. Lau, Q. Liu, A. P. Paulikas, C.-J. Sun, Z. Cai, J. R. Guest, Y. Ren, V. Stamenkovic, L. A. Curtiss, Y. Liu, T. Rajh. Facet-Dependent Active Sites of a Single Cu_2O Particle Photocatalyst for CO_2 Reduction to Methanol. *Nat. Ener.* **2019**, *4*, 957.

5. Y. Yuan, K. He, B. W. Byles, **C. Liu**, K. Amine, J. Lu, E. Pomerantseva, R. Shahbazian-Yassar. Deciphering the Atomic Patterns Leading To MnO_2 Polymorphism. *Chem* **2019**, *5*(7), 1793.

6. F. Liu, **C. Liu**, X. Zhong. Enhancing Electrocatalysis for Hydrogen Production over CoP Catalyst by Strain: A Density Functional Theory Study. *Phys. Chem. Chem. Phys.*, **2019**, *21*, 9137.

7. G. Tan, L. Chong, C. Zhan, J. Wen, L. Ma, Y. Yuan, X. Zeng, F. Guo, J. E. Pearson, T. Li, T. Wu, D. Liu, R. Shahbazian-Yassar, J. Lu, **C. Liu**,***** K. Amine. Insights into Structural Evolution of Lithium Peroxides with Reduced Charge Overpotential in $Li{-}O_2$ System. *Adv. Energy Mater.* **2019**, 1900662.

8. Z. H. Syed, D. M. Kaphan, F. A. Perras, M. Pruski, M. S. Ferrandon, E. C. Wegener, G. Celik, J. Wen, **C. Liu**, F. Dogan, K. I. Goldberg, M. Delferro. Electrophilic Organoiridium(III) Pincer Complexes on Sulfated Zirconia for Hydrocarbon Activation and Functionalization. *J. Am. Chem. Soc.* **2019**, *141*(15), 6325.

9. Y. Yuan, **C. Liu**, B. W. Byles, W. Yao, B. Song, M. Cheng, Z. Huang, K. Amine, J. Lu, E. Pomerantseva, R. Shahbazian-Yassar. Ordering Heterogeneity of [MnO_6] Octahedra in Tunnel-structured MnO_2 and Its Influence on Ion Storage. *Joule* **2019**, *3*(2), 471.

10. S. Dong, W. Shin, H. Jiang, X. Wu, Z. Li, J. Holoubek, W. F. Stickle, **C. Liu**, J. Lu, P. A. Greaney, X. Zhang, X. Ji. Ultra-fast NH_4^+ Storage: Strong H Bonding between NH_4^+ and Bi-layered V_2O_5. *Chem* **2019**, *5*(6), 1537.

11. M. Asadi, M. H. Motevaselian, T. V. Sun, **C. Liu**, P. Abbasi, A. Moradzadeh, P. Zapol, A. Khodadoust, L. A. Curtiss, N. R. Aluru, A. Salehi-Khojin. CO_2 Photo-reduction at 23% Efficiency Using Inexpensive and Earth Abundant Catalytic System. *Adv. Energy Mater.* **2019**, *9*, 1803536.

12. C. Plascencia, L. A. Curtiss, **C. Liu**.* Computational Studies of Silica Supported Metal Ions for Hydrogen Activation: Catalytic Properties of Metals and Performance of DFT Functionals. *J. Phys. Chem. A* **2019**, *123* (1), 171.

13. J. Camacho-Bunquin, M. Ferrandon, H. Sohn, D. Yang, J. Kropf, C. Yang, J. Wen, **C. Liu**, P. A. Ignacio-de Leon, H. Kim, F. A. Perras, M. Pruski, C. L. Marshall, P. C. Stair, M. Delferro. Atomically Precise Strategy to Sub-Nanometer PtZn Alloy Catalyst for Deep Dehydrogenation of n-Butane to 1,3-Butadiene. *ACS Catal.* **2018**, *8*, 10058-10063.

14. Y. Yuan, G. Tan, J. Wen, J. Lu, L. Ma, **C. Liu**, X. Zuo, R. Shahbazian-Yassar, T. Wu, K. Amine. Encapsulating Various Sulfur Allotropes within Graphene Nanocages for Long-Lasting Lithium Storage. *Adv. Funct. Mater.* **2018**, 1706443.

15. **C. Liu**,* J. Camacho-Bunquin, M. Ferrandon, A. Savara, H. Sohn, D. Yang, D. Kaphan, P. Anne Ignacio-de Leon, S. Liu, U. Das, B. Yang, A. S. Hock, P. C. Stair, L. A. Curtiss, and M. Delferro. Development of Activity-Descriptor Relationships for Supported Metal Ion Hydrogenation Catalysts on Silica. *Polyhedron*, **2018**, *152*, 73. (**Invited Paper**)

16. A. Halder, **C. Liu**, Z. Liu, J. D. Emery, M. J. Pellin, L. Curtiss, P. Zapol, S. Vajda, A.B.F. Martinson. Water Oxidation Catalysis via Size-Selected Iridium Clusters. *J. Phys. Chem. C.*, **2018**, *122* (18), 9965.

17. R. R. Langeslay, H. Sohn, B. Hu, J. S. Mohar, M. Ferrandon, **C. Liu**, H. Kim, J. Niklas, O. Plouektov, E. E. Alp, A. P. Sattelberger, A. S. Hocka, M. Delferro. Nuclearity Effects in Supported, Single-Site Fe(II) Hydrogenation Catalysts. *Dalton Trans.*, **2018**, *47*, 10842.

18. R. C. Klet, D. M. Kaphan, **C. Liu**, F. A. Perras, M. Pruski, A. S. Hock, M. Delferro. Evidence for Redox Mechanisms in Organometallic Chemisorption and Reactivity on Sulfated Metal Oxides. *J. Am. Chem. Soc.*, **2018**, *140* (20), 6308.

19. M. Asadi, B. Sayahpour, P. Abbasi, A. T. Ngo, K. Karis, J. R. Jokisaari, **C. Liu**, B. Narayanan, M. Gerard, P. Yasaei, X. Hu, A. Mukherjee, K. Chun Lau, R. S. Assary, F. Khalili-Araghi, R. F. Klie, L. A. Curtiss, A. Salehi-Khojin. Enabling Operation of Lithium-Oxygen Batteries with Long Cycle Life in a Realistic Air Atmosphere. *Nature*, **2018**, *555*, 502.

20. J. Camacho-Bunquin, M. Ferrandon, H Sohn, D. Yang, **C. Liu**, P. A. Ignacio-de Leon, F. A. Perras, M. Pruski, P. C. Stair, and M. Delferro. Chemoselective Hydrogenation with Supported Organoplatinum(IV) Catalyst on Zn(II)/SiO_2. *J. Am. Chem. Soc*., **2018**, *140* (11), 3940.

21. H. Sohn, J. Camacho-Bunquin, R. R. Langeslay, P. A. A. Ignacio-de Leon, J. Niklas, O. G. Poluektov, **C. Liu**, J. G. Connell, D. Yang, A. J. Kropf, H. Kim, P. C Stair, M. Ferrandon and M. Delferro. Isolated, Well-defined Organovanadium(III) on Silica: Single-site Catalyst for Hydrogenation of Alkenes and Alkynes. *Chem. Commun.*, **2017**, *53*, 7325.

22. G. Tan, R. Xu, Z. Xing, Y. Yuan, J. Lu, J. Wen, **C. Liu**, L. Ma, C. Zhan, Q. Liu, T. Wu, Z. Jian, R. Shahbazian-Yassar, Y. Ren, D. J. Miller, L. A. Curtiss, X. Ji, K. Amine. Burning Lithium in CS_2 for High-performing Compact Li_2S-graphane Nanocapsules for Li-S Batteries. *Nat. Ener.* **2017**, *2*, 17090.

23. B. Yang,[#] **C. Liu**,[#] A. Halder, E. Tyo, A.B.F. Martinson, S. Seifert, P. Zapol, L. A. Curtiss, S. Vajda. Copper Cluster Size Effect in Methanol Synthesis from CO_2. *J. Phys. Chem. C.* **2017**, *121* (19), 10406.

24. G. Tan, L. Chong, R. Amine, J. Lu, **C. Liu**, Y. Yuan, J. Wen, K. He, X. Bi, Y. Guo, H.-H. Wang, R. Shahbazian-Yassar, S. A. Hallaj, D. J. Miller, D. Liu, K. Amine. Toward Highly Efficient Electrocatalyst for Li–O_2 Batteries Using Biphasic N-Doping Cobalt@Graphene Multiple-Capsule Heterostructures. *Nano Lett.* **2017**, *17* (5), 2959.

25. Z.Qi, C. Xiao, **C. Liu**, T. W. Goh, L. Zhou, R. Maligal-Ganesh, Y. Pei, X. Li, L. A. Curtiss, and W. Huang. Sub-4 nm PtZn Intermetallic Nanoparticles for Enhanced Mass and Specific Activities in Catalytic Electro-Oxidation Reaction. *J. Am. Chem. Soc.* **2017**, *139* (13), 4762.

26. J. Camacho-Bunquin, M. Ferrandon, U. Das, F. Dogan, **C. Liu**, C. Larsen, A. E. Platero-Prats, L. A. Curtiss, A. Hock, J. Miller, S. Nguyen, C. Marshall, M. Delferro, P. Stair. Supported Aluminum Catalysts for Olefin Hydrogenation. *ACS Catal*., **2017**, *7* (1), 689.

27. P. Abbasi, M. Asadi, **C. Liu**, S. S. Sharifi-Asl, A. Behranginia, B. Sayahpour, P. Zapol, R. S. Yassar, L. A. Curtiss, A. Salehi-Khojin. Tailoring the Edge Structure of Molybdenum Disulfide toward Electrocatalytic Reduction of Carbon Dioxide. *ACS Nano*, **2017**, *11* (1), 453.

28. M. Asadi, K. Kim,[#] **C. Liu**,[#] V. A. Addepalli, P. Phillips, P. Abbasi, A. Behranginia, P. Yasaei, R. Haasch, P. Zapol, B. Kumar, R. F. Klie, J. Abiade, L. A. Curtiss, A. Salehi-Khojin. Nanostructured Transition Metal Dichalcogenide Electrocatalysts for CO_2 Reduction in Ionic Liquid. *Science*, **2016**, *353* (6298), 467.

29. M. Asadi, B. Kumar, **C. Liu**, P. Phillips, P. Yasaei, A. Behranginia, P. Zapol, R. F. Klie, L. A. Curtiss, A. Salehi-Khojin. A Molybdenum Disulfide/Ionic Liquid Co-catalyst for Lithium–Oxygen Batteries. *ACS Nano*, **2016**, *10* (2), 2167.

30. A. Behranginia, M. Asadi, **C. Liu**, P. Yasaei, B. Kumar, P. Phillips, T. Foroozan, J. C. Waranius, J. Abiade, R. F. Klie, L. A. Curtiss, A. Salehi-Khojin. Highly Efficient Hydrogen Evolution Reaction Using Crystalline Layered Three Dimensional Molybdenum Disulfides Grown on Graphene Film. *Chem. Mater.*, **2016**, *28* (2), 549.

31. **C. Liu**, T. J. Evans, L. Cheng, M. R. Nimlos, C. Mukarakate, D. J. Robichaud, R. S. Assary, L. A. Curtiss. Catalytic Upgrading of Biomass-Derived Compounds via C-C Coupling Reactions: Furan and Acetaldehyde Reactions in HZSM-5. *J. Phys. Chem. C.* **2015**, *119* (42), 24025.

32. **C. Liu**, B. Yang, E. Tyo, S. Seifert, J. E. Ernst, B. von Issendorff, P. Zapol, S. Vajda, L. A. Curtiss. Carbon Dioxide Conversion to Methanol over Size-selected Cu_4 Clusters at Low Pressures. *J. Am. Chem. Soc.*, **2015**, *137* (27), 8676.

33. **C. Liu**, A. K. Wilson. Cleavage of the β-O-4 Linkage of Lignin using Group 8 Pincer Complexes: A DFT Study. *J. Mol. Catal. A: Chem.*, **2015**, *399*, 33.

34. **C. Liu**, R. S. Assary, L. A. Curtiss. Investigation of Thermochemistry Associated with the Carbon–Carbon Coupling Reactions of Furan and Furfural Using ab Initio Methods. *J. Phys. Chem. A*, **2014**, *118* (25), 4392.

35. **C. Liu**, H. He, P. Zapol, L. A Curtiss. Computational Studies of Electrochemical CO_2 Reduction on Subnanometer Transition Metal Clusters. *Phys. Chem. Chem. Phys.*, **2014**, *16*, 26584. (**Invited Paper**)

36. M. R. Jones, **C. Liu**, A. K. Wilson. "Molecular Dynamics Studies of the Protein–Protein Interactions in Inhibitor of κB Kinase-β" *J. Chem. Inf. Model*., **2014**, *54* (2), 562.

37. **C. Liu**, T. R. Cundari, A. K. Wilson. Periodic Trends in 3d Metal Mediated CO_2 Activation. *Applications of Molecular Modeling to Challenges in Clean Energy*. January 1, **2013**, 67. (**Invited Book Chapter**)

38. **C. Liu**, C. Peterson, A. K. Wilson. C-O Bond Cleavage of Dimethyl Ether by Transition Metal Ions: A Systematic Study on Catalytic Properties of Metals and Performance of DFT Functionals. *J. Phys. Chem. A*, **2013**, *117* (24), 5140.

39. **C. Liu**, T. R. Cundari, A. K. Wilson. Reduction of CO_2 to CO on Transition Metal Surfaces: In Comparison with Homogeneous Catalysis. *J. Phys. Chem. C*, **2012**, *116* (9), 5681.

40. **C. Liu**, T. R. Cundari, A. K. Wilson. Reaction Mechanism of the Reverse Water-gas Shift Reaction Using First-row Middle Transition Metal Catalysts L'M(M: Fe, Mn, Co): A Computational Study. *Inorg. Chem.*, **2011**, *50* (18), 8782.

41. **C. Liu**, L. Munjanja, T. R. Cundari, A. K. Wilson. Theoretical Studies on the Catalysis of the Reverse Water Gas Shift Reaction Using First-row Transition Metal β-diketiminato Complexes. *J. Phys. Chem. A.* **2010**, *114*, 6207.

42. E. Gao, **C. Liu**, M. Zhu, H. Lin, Q. Wu, L. Liu. Current Development of Pd(II) Complexes as Potential Antitumor Agents. *Anticancer Agents Med. Chem.* **2009**, *9* (3), 356.

43. E. Gao, Q. Wu, **C. Liu**, F. Liu, H. Liu. Syntheses and DNA-Binding Study of the Zinc (II) Complex with 2,5-Thiophenedicarboxylic Acid. *J. Chin. Clin. Med.* **2008**, *3* (8), 442.

PRESENTATIONS AND WORKSHOPS

1. "Computational Design and Characterization of Catalysts from First Principles, Multiscale Modeling and Data Science", Chemical Sciences and Engineering Division Retreat, Argonne National Laboratory, February 2020. **(Invited)**

2. "Development of Silica Supported Single-Site Metal Ion Catalysts for Alkenes Hydrogenation and Alkanes Dehydrogenation", Department of Energy (DOE) Catalysis Program Principle Investigator Meeting, July 2019. **(Invited)**

3. "From Understanding Reaction Mechanism to Designing Better Catalysts and Catalytic Processes", 2019 North American Catalysis Society Meeting, June 2019.

4. "Computational Catalyst Design", Armour College of Engineering, Illinois Institute of Technology, Jan. 2019. **(Invited Lecture)**

5. "Computational Studies of Bimetallic Nano-Cluster for Non-Oxidative Dehydrogenation of Light Alkanes", Department of Energy (DOE) Catalysis Program Principle Investigator Meeting, July 2018. **(Invited)**

6. "Computational Design of Supported Single-site Catalysts for Alkene Hydrogenation", University of Notre Dame, Nov. 2017. **(Invited)**

7. Workshop: Innovations in Materials Science, University of Delaware, Oct. 2017. **(Invited)**

8. "Discovery of Active Single-atom Heterogeneous Catalysts for Alkene Hydrogenation via the Development of Activity-descriptor Relationships", Department of Energy (DOE) Catalysis Program Principle Investigator Meeting, July 2017. **(Invited)**

9. "Computational Studies of Catalysts for Energy", California State University, Fullerton, Feb. 2016. **(Invited)**

10. "Computational Catalyst Design for Renewable Energy: Catalytic Reduction of CO_2 to CO and Fuels", Auburn University, Feb. 2016. **(Invited)**

11. "Novel Catalysts for Renewable Energy from Theoretical Predictions", University of California, Merced, Feb. 2016. **(Invited)**

12. "Computational Catalyst Design for Renewable Energy: Catalytic Reduction of Carbon Dioxide", University of Colorado, Boulder, Feb. 2016. **(Invited)**

13. "Catalyst Design for Renewable Energy using First-principle Calculations", Northeastern University, Jan. 2016. **(Invited)**

14. "Computational Studies of Catalysis for Renewable Energy: Catalytic Reduction of CO_2 to CO and Fuels", California State University, Los Angeles, Jan. 2016. **(Invited)**

15. "Computational Catalyst Design for Sustainable Energy", University of California, Santa Cruz, Dec. 2015. **(Invited)**

16. "In Silico Zeolite Catalyzed Carbon-Carbon Coupling Reactions for Furan Upgrading", 249th ACS National Meeting, March 2015. **(Invited)**

17. "Computational Studies of Electrochemical Reduction of CO_2 to CO using Transition Metal Dichalcogenide Nanoflakes", 253rd ACS National Meeting, April 2017.

18. "Trends of SiO_2 Supported Single-site Catalysts for Alkene Hydrogenation based on Combined DFT and Experimental Studies", 253rd ACS National Meeting, April 2017.

19. "Computational Studies of Doping and Dissolution in Lithium Transition Metal Oxides", 2016 MRS Spring Meeting & Exhibit, March 2016.

20. "Computational Studies of Chemical and Electrochemical CO_2 Reduction: From Metals Surfaces and Metal Clusters to Semiconductors", 250th ACS National Meeting, August 2015.

21. "Electronchemical Reduction of CO_2 to Fuels using Supported Transition Metal Clusters: Comparison with Gas-Phase Reactions" 248th ACS National Meeting, August 2014.

22. "Computational Studies of C-C Coupling to Increase the Carbon Content of Furans with Zeolite Catalysts" 247th ACS National Meeting, March 2014.

23. "Transition Metal Catalyst Mediated C-O Bond Activation of the β-O-4 Linkage of Lignin", 245th ACS National Meeting, April 2013.

24. "C-O Bond Cleavage Using Transition Metal Catalysts: From Dimethyl Ether Activation To Lignin Degradation", 245th ACS National Meeting, April 2013.

25. "Transition Metal Catalysts Mediated C-O Bond Cleavage of β-O-4 Linkage of Lignin", Southwest Theoretical Chemistry Conference, October 2012.

26. "Computational Studies of CO_2 Activation and Conversion using 3*d* Transition Metal Catalysts", International Conference of Quantum Chemistry, June 2012.

27. "Computational Studies on Transition Metal Catalysts Mediated CO_2 Activation", 45th ACS Meeting in Miniature DFW Section, April 2012.

28. "Computational Studies on CO_2 Activation using Transition Metal Catalysts: In Consideration of Homogeneous and Heterogeneous Catalysis", 243th ACS National Meeting, March 2012.

29. "DFT Studies on CO_2 Activation using Homogeneous and Heterogeneous Transition Metal Catalysts", 24th Austin Symposium on Molecular Structure and Dynamics at Dallas, March 2012.

30. "CO_2 Activation by Transition Metal Catalysts: In Consideration of Homogeneous and Heterogeneous Catalysis", 2011 Southwest Theoretical Chemistry Conference, October 2011.

31. "CO_2 Reduction on Transition Metal Surfaces: A Computational Study", American Conference of Theoretical Chemistry, July 2011.

32. "Reaction Mechanism of the Reverse Water-gas Shift Reaction Using Transition Metal Catalysts L'M (L': β-diketiminate, M: Fe, Mn, Co): A Computational Study", 44th ACS Annual Meeting in Miniature DFW Section, April 2011.

33. "Computational Studies of CO_2 Activation and Conversion Using Transition Metal β-diketiminato Complexes", Southwest Theoretical Chemistry Conference, October 2010.

34. "Thermodynamics and Kinetics of CO_2 Activation using Middle Transition Metal Complexes", The Chemistry Centennial Celebration, University of North Texas, October 2010.

35. "Theoretical Studies of the Activation of Carbon Dioxide Using Transition Metal β-diketiminato Complexes", 240th ACS National Meeting, August 2010.

36. "Modeled Mechanism of the Reverse Water Gas Shift Reaction Using Transition Metal catalysts", ACS Summer School on Green Chemistry and Sustainable Energy, July 2010.

37. "Theoretical Studies on the Catalysis of the Reverse Water Gas Shift Reaction Using Transition Metal β-diketiminato Complexes", 43rd Annual Meeting in Miniature, April 2010.

38. "β-diketiminato catalysts and their potential role in CO_2 activation", 239th ACS National Meeting, March 2010.