Shaama Mallikarjun Sharada

Assistant Professor of Chemical Engineering and Materials Science and Chemistry

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EDUCATION

University of California, Berkeley (2010-15)
- Ph.D. in Chemical Engineering (Minor: Physical Chemistry)
- Dissertation title: "Development of a hessian-free algorithm for transition state searches, application to reactions of light alkanes in zeolite catalysts, and extension to wavefunction stability analysis in the absence of analytical hessians."
- Advisors: Prof. Alexis T. Bell & Prof. Martin Head-Gordon

Indian Institute of Technology, Bombay, India (2003-08)
- B.Tech. and M.Tech. in Chemical Engineering
- Recipient: Institute Gold Medal & Institute Silver Medal

PROFESSIONAL EXPERIENCE

WiSE Gabilan Assistant Professor of Chemical Engineering & Materials Science (2017 – Present)
University of Southern California, Los Angeles CA

Assistant Professor of Chemistry (Courtesy) (2020 – Present)
University of Southern California, Los Angeles CA

Post-doctoral Researcher, Chemical Engineering (2015 –2017)
Stanford University
Advisors: Prof. Jens Nørskov, Prof. Thomas Bligaard

Developer (2011 – 2015)
Q-Chem Inc., ab initio quantum chemistry software

Business Analyst (2008 – 2010)
A T Kearney India Ltd., Management consulting

Visiting Scientist (Spring 2008)
Max Planck Institute, Magdeburg, Germany

Young Engineering Fellow (Summer 2006)
Indian Institute of Science, Bangalore, India

HONORS AND AWARDS

External
- Invitee, Telluride Workshop on Exploring Nitrogen Activation Mechanisms (2021)
- Scialog Fellow, Negative Emissions Science, RCSA & Alfred P. Sloan Foundation (2020, 21)
- Outstanding Young Engineer Award, Orange County Engineering Council (2020)
- Doctoral New Investigator, American Chemical Society Petroleum Research Fund (2020)

USC
- Chevron Research Innovation Award, USC Viterbi (Inaugural) (2022)
- Zumberge Individual Award, USC (2019)
- WiSE Gabilan Jr. Chair, USC (2017)

Prior to USC
- Kokes Award, 24th North American Catalysis Society (2015)
- Invitee, 128th International Summer Course, BASF, Ludwigshafen (2014)
- Institute Gold Medal, Institute Silver Medal, Indian Institute of Technology Bombay (2008)
- Young Engineering Fellowship, Indian Institute of Science Bangalore (2006)
- IIT Bombay Heritage Fund Scholarship (2006)

RESEARCH INTERESTS

Development and application of quantum chemistry and ab initio molecular dynamics methods to understand quantum, variational, and dynamical effects in catalysis to design sustainable reaction pathways with molecular, heterogeneous, and photoredox catalysts.

PEER REVIEWED JOURNAL PUBLICATIONS

Google Scholar: https://scholar.google.com/citations?user=U6IAZYgAAAAJ&hl=en
Web of Science/Publons: https://publons.com/researcher/1316430/shaama-mallikarjun-sharada/

Note: My name is highlighted in bold, and my students' names have **, *, $^{+}$, or $^{\#}$ after them for Postdoc, PhD, Masters, and undergraduate/high school students, respectively. Corresponding authors are underlined. Hyperlinks provided where available. (IF = Impact factor)

Book chapter

1. "Transition structures, reaction paths, and kinetics: Methods and applications in catalysis," Bac, S.*; Lan, Z.*; **Mallikarjun Sharada, S**. In Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, **2022**, *Elsevier*. https://doi.org/10.1016/B978-0-12-821978-2.00006-4

Articles in preparation

2. "Substituent effects on CO_2 capture by anilines: A combined spectroscopic and computational study," Delibas, B.; Kron, K. J.*; Salazar, N.; Cotton, D. E.; **Mallikarjun Sharada, S.**; Dawlaty, J. M.

Peer-reviewed Journal Publications

USC

3. "Thermochemical reduction yields novel iron nanophase during decomposition of the perovskite $CaTi_{1-x}Fe_xO_{3-\delta}$," Luong, J.; Tsung, A.$^{\#}$; Humphrey, N.*; Guo, H.; Lam, B.; **Mallikarjun Sharada, S.**, Bowman, W. J. **2022**, *Under review.*
4. "Controlling Selectivity for Dechlorination of Poly(Vinyl Chloride) with (Xantphos)RhCl," Bush, N.; Assefa, M.; Bac, S.*; **Mallikarjun Sharada, S.**, Fieser, M. **2022**, *Under review.*
5. "Recent advances towards efficient calculation of higher nuclear derivatives in quantum chemistry," Bac, S.*; Patra, A.**; Kron, K. J.*; **Mallikarjun Sharada S.**, **2022**, The Journal of Physical Chemistry A, *Accepted.* https://doi.org/10.1021/acs.jpca.2c05459
6. "A computational mechanistic study of CH hydroxylation with mononuclear copper-oxygen complexes," Lan, Z.*; Toney, J.$^{\#}$; **Mallikarjun Sharada, S.** (Emerging Investigator Series) **2022**, Catalysis Science and Technology, *Accepted*. https://doi.org/10.1039/D2CY01128J
7. "Toward efficient direct dynamics studies of chemical reactions: A novel matrix completion algorithm," Quiton, S. J. $^{\#}$; Chae, J.; Bac, S.*; Kron, K. J.*; Mitra, U., **Mallikarjun Sharada, S.** **2022**, Journal of Chemical Theory and Computation, *18*, 4327-4341. https://doi.org/10.1021/acs.jctc.2c00321
8. "A matrix completion algorithm for efficient calculation of quantum and variational effects in chemical reactions," Bac, S.*; Quiton, S. J.$^{\#}$; Kron, K. J.*; Chae, J.; Mitra, U., **Mallikarjun Sharada, S.** (Emerging Investigators Special Issue) **2022**, The Journal of Chemical Physics, *156*, 184119. https://doi.org/10.1063/5.0091155
9. "Organic photoredox catalysts for CO_2 reduction: Driving discovery with genetic algorithms," Kron, K. J.*; Rodriguez-Katakura, A.$^{\#}$; Regu, P.$^{+}$; Reed, M. N.$^{\#}$; Elhessen, R.$^{\#}$; **Mallikarjun Sharada, S.** (Chemical design by artificial intelligence) **2022**, The Journal of Chemical Physics, *156*, 184109. https://doi.org/10.1063/5.0088353
10. "Modeling and characterization of exciplexes in photoredox cycles for CO_2 reduction: Insights from quantum chemistry and fluorescence spectroscopy," Kron, K. J.*; Hunt, J. R.; Dawlaty, J. M.; **Mallikarjun Sharada, S**. **2022**, The Journal of Physical Chemistry A, *126*, 2319-2329. https://doi.org/10.1021/acs.jpca.1c10658

11. "Kinetic and mechanistic details of bulk ZnO dissolution using a thiol-imidazole system," Koskela, K. M.; Quiton, S. J.[#]; **Mallikarjun Sharada, S.**; Williams, T. J., Brutchey, R. L., **2022**, Chemical Science, **2022**, *13*, 3208-3215. https://doi.org/10.1039/D1SC06667F
12. "A computational study of the mechanism of chloroalkane dechlorination with Rh(I) complexes," Bac, S.*; Fieser, M. E.; **Mallikarjun Sharada, S.** Physical Chemistry Chemical Physics, **2022**, *24*, 3518-3522. https://doi.org/10.1039/D1CP03949K
13. "CO oxidation with atomically dispersed catalysts: Insights from the energetic span model," Bac, S.*; **Mallikarjun Sharada, S.** ACS Catalysis, **2022**, *12*, 2064-2076. https://doi.org/10.1021/acscatal.1c04299
14. "Photoredox Chemistry with Organic Catalysts: Role of Computational Methods," Kron, K. J.*; Rodriguez-Katakura, A.[#]; Elhessen, R.[#]; **Mallikarjun Sharada, S.** ACS Omega, **2021**, 6, 33253-33264. https://doi.org/10.1021/acsomega.1c05787
15. "Perspective and Challenges in Electrochemical Approaches for Reactive CO_2 Separations," Gurkan, B.; Su, X.; Klemm, A.; Kim, Y.; **Mallikarjun Sharada, S.**; Rodriguez-Katakura, A.[#]; Kron, K. J.* iScience, **2021**, 103422. https://doi.org/10.1016/j.isci.2021.103422
16. "Probing the ligand exchange of N-heterocyclic carbene-capped Ag_2S nanocrystals with amines and carboxylic acids," Smock, S. R.; Alimento, R.[#]; **Mallikarjun Sharada, S.**, Brutchey, R. L. Inorganic Chemistry, **2021**, *60*, 13699-13706. https://doi.org/10.1021/acs.inorgchem.1c02018
17. "Adsorbate-assisted migration of the metal atom in atomically dispersed catalysts: An ab initio molecular dynamics study," Humphrey, N.*; Bac, S.*; **Mallikarjun Sharada, S.** The Journal of Chemical Physics, **2021**, *154*, 234709. https://doi.org/10.1063/5.0054991
18. "A framework for constructing linear free energy relationships to design molecular transition metal catalysts," Lan, Z.*; **Mallikarjun Sharada, S.** (Emerging Investigators Special Issue) Physical Chemistry Chemical Physics, **2021**, *23*, 15543-15556. https://doi.org/10.1039/D1CP02278D
19. "Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package," Epifanovsky, E.; Gilbert, A.; ...; **Mallikarjun Sharada, S.** ...; Krylov, A., The Journal of Chemical Physics, **2021**, *155*, 084801. https://doi.org/10.1063/5.0055522
20. "Consistent inclusion of continuum solvation in energy decomposition analysis: Theory and application to molecular CO_2 reduction catalysts," Mao, Y.; Loipersberger, M.; Kron, K. J.*; Derrick, J.; Chang, C.; **Mallikarjun Sharada, S.**; Head-Gordon, M., Chemical Science, **2021**, *12*, 1398-1414. https://doi.org/10.1039/D0SC05327A
21. "Ab initio molecular dynamics reveals new metal-binding sites in atomically dispersed Pt_1/TiO_2 catalysts," Humphrey, N.*; Bac, S.*; **Mallikarjun Sharada, S.**, The Journal of Physical Chemistry C, **2020**, *124*, 24187-24195. https://doi.org/10.1021/acs.jpcc.0c06771
22. "A matrix completion algorithm to recover modes orthogonal to the minimum energy path in chemical reactions," Quiton, S. J.[#]; Mitra, U.; **Mallikarjun Sharada, S.** (Women in Physical Chemistry & Chemical Physics Special Issue) The Journal of Chemical Physics, **2020**, *153*, 054122. https://doi.org/10.1063/5.0018326
23. "Heterobimetallic complexes of IrM (M = Fe^{II}, Co^{II}, and Ni^{II}) core and bridging 2-(diphenylphosphino) pyridine: Electronic structure and electrochemical behavior," Cherepakhin, V.; Hellman, A.; Lan, Z.*; **Mallikarjun Sharada, S.**; Williams, T. J. Dalton Transactions, **2020**, *49*, 10509-10515. https://doi.org/10.1039/D0DT01801E
24. "Computational analysis of electron transfer kinetics for CO_2 reduction with organic photoredox catalysts," Kron, K. J.*; Gomez, S. J.[#]; Mao, Y.; Cave, R. J.; **Mallikarjun Sharada, S.**, Journal of Physical Chemistry A, **2020**, *124*, 5359-5368. https://doi.org/10.1021/acs.jpca.0c03065
25. "Linear free energy relationships for transition metal chemistry: Case study of CH activation with copper-oxygen complexes," Lan, Z.*; **Mallikarjun Sharada, S.** ***HOT Article***, Physical Chemistry Chemical Physics, **2020**, *22*, 7155-7159. https://doi.org/10.1039/D0CP01245A
26. "Synthesis and electrocatalytic HER studies of carbene-ligated $Cu_{3-x}P$ nanocrystals," Tappan, B.; Chen, K.; Lu, H.; **Mallikarjun Sharada, S.**; Brutchey, R. ACS Applied Materials & Interfaces, **2020**, *2*, 16394-16401. https://doi.org/10.1021/acsami.0c00025
27. "A new mechanism of metal-ligand cooperative catalysis in transfer hydrogenation of ketones," Demianets, I.; Cherepakhin, V.; Maertens, A.; Lauridsen, P. J.; **Mallikarjun Sharada, S.**; Williams, T. J. Polyhedron, **2020**, *182*, 114508. https://doi.org/10.1016/j.poly.2020.114508

28. "Computational strategies to probe CH activation in dioxo-dicopper complexes," Lan, Z.*; **Mallikarjun Sharada, S.** ***HOT Article***, Physical Chemistry Chemical Physics, **2018**, *20*, 25602-25614. https://doi.org/10.1039/C8CP05096A

Prior to USC

29. "Adsorption on transition metal surfaces: Transferability and accuracy of DFT using the ADS41 dataset," **Mallikarjun Sharada, S.**; Karlsson, R. K. B.; Maimaiti, Y.; Voss, J.; Bligaard, T. Physical Review B, **2019**, *100*, 035409. https://doi.org/10.1103/PhysRevB.100.035439
30. "A theoretical study of the effect of a non-aqueous proton donor on electrochemical ammonia synthesis," Zhang, L.; **Mallikarjun Sharada, S.**; Singh, A. R.; Rohr, B. A.; Su, Y.; Qiao, L.; Nørskov, J. K. Physical Chemistry Chemical Physics, **2018**, *20*, 4982-4989. https://doi.org/10.1039/C7CP05484J
31. "SBH10: A benchmark database of barrier heights on transition metal surfaces," **Mallikarjun Sharada, S.**; Bligaard, T.; Luntz, A. C.; Kroes, G.-J.; Nørskov, J. K. ***ACS Editors' Choice***, Journal of Physical Chemistry C, **2017**, *121*, 19807-19815. https://doi.org/10.1021/acs.jpcc.7b05677
32. "Theoretical analysis of the influence of pore geometry on monomolecular cracking and dehydrogenation of n-butane in Bronsted-acid zeolites," Van der Mynsbrugge, J.; Janda, A.; **Mallikarjun Sharada, S.**; Lin, L-C.; Van Speybroeck, V.; Head-Gordon, M.; Bell, A. T. ACS Catalysis, **2017**, *7*, 2685-2697. https://doi.org/10.1021/acscatal.6b03646
33. "Ethane and propane dehydrogenation over PtIr/Mg(Al)O," Wu, J.; **Mallikarjun Sharada, S.**; Ho, C.; Hauser, A. W.; Head-Gordon, M.; Bell, A. T. Applied Catalysis A: General, **2015**, *506*, 25-32. https://doi.org/10.1016/j.apcata.2015.08.029
34. "Wavefunction stability analysis without analytical electronic hessians: Application to orbital-optimized second order Møller-Plesset theory and VV10-containing density functionals," **Mallikarjun Sharada, S.**; Stuck, D.; Sundstrom, E. J.; Bell, A. T.; Head-Gordon, M. Molecular Physics, **2015**, *113*, 1802-1808. https://doi.org/10.1080/00268976.2015.1014442
35. "Adsorption thermodynamics and intrinsic activation parameters for monomolecular cracking of n-alkanes on Brønsted acid sites in zeolites," Janda, A.; Vlaisavljevich, B.; Li, L-C; **Mallikarjun Sharada, S.**; Smit, B.; Head-Gordon, M.; Bell, A. T. Journal of Physical Chemistry C, **2015**, *119*, 10427-10438. https://doi.org/10.1021/acs.jpcc.5b01715
36. "Improved force field parameters for QM/MM simulations of the energies of adsorption for molecules in zeolites and a free rotor correction to the rigid rotor harmonic oscillator model for adsorption enthalpies," Li, Y-P.; Gomes, J.; **Mallikarjun Sharada, S.**; Bell, A. T.; Head-Gordon, M. Journal of Physical Chemistry C, **2015**, *119*, 1840-1850. https://doi.org/10.1021/jp509921r
37. "Advances in molecular quantum chemistry contained in the Q-Chem 4 program package," Shao, Y.; Gan Z.; Epifanovsky, E.; ...; **Mallikarjun Sharada, S.** ...; Head-Gordon, M. Molecular Physics, **2015**, *113*, 184-215. https://doi.org/10.1080/00268976.2014.952696
38. "A finite difference Davidson procedure to sidestep full ab initio hessian calculation: Application to characterization of stationary points and transition state searches," **Mallikarjun Sharada, S.**; Bell, A. T.; Head-Gordon, M. The Journal of Chemical Physics, **2014**, *140*, 164115. https://doi.org/10.1063/1.4871660
39. "Insights into the kinetics of cracking and dehydrogenation reactions of light alkanes in H-MFI," **Mallikarjun Sharada, S.**; Zimmerman, P. M.; Bell, A. T.; Head-Gordon, M. Journal of Physical Chemistry C, **2013**, *117*, 12600-12611. https://doi.org/10.1021/jp402506m
40. "Automated transition state searches without evaluating the hessian," **Mallikarjun Sharada, S.**; Zimmerman, P. M.; Bell, A. T.; Head-Gordon, M. Journal of Chemical Theory and Computation, **2012**, *8*, 5166-5174. https://doi.org/10.1021/ct300659d
41. "A comprehensive single-particle model for solid-state polymerization of poly(L-lactic acid)," Katiyar, V.; **Mallikarjun Sharada, S.**; Nanavati, H. Journal of Applied Polymer Science, **2011**, *122*, 2966-2980. https://doi.org/10.1002/app.34061
42. "Degradation of water soluble polymers under combined ultrasonic and ultraviolet radiation," Aarthi, T.; **Mallikarjun Sharada, S.**; Madras, G. Industrial and Engineering Chemistry Research, **2007**, *46*, 6204-6210. https://doi.org/10.1021/ie070287

INVITED TALKS AND SEMINARS

Invited departmental/research/society seminars

1. "Catalyst discovery for metal-free, photoredox CO_2 reduction," Seminars on Theory and Simulation of Electronic and Optical Processes in Molecules and Materials (Virtual) 05/2022
2. "The pursuit of free energies and free energy relationships," Department Seminar, Chemistry, University of Chicago 05/2022
3. "The pursuit of free energies and free energy relationships," Department Seminar, Chemical Engineering, University of Washington 04/2022
4. "Catalyst discovery for metal-free, photoredox CO_2 reduction," Greater Boston Area Theoretical Chemistry Seminar (Virtual) 03/2022
5. "Dynamical evolution of atomically dispersed catalysts," Department Seminar, Materials Science and Engineering, University of California at Irvine 03/2022
6. "Modeling photoredox pathways for CO_2 reduction", Department Seminar, Chemistry, University of Oklahoma (Virtual) 02/2022
7. "The pursuit of free energies and free energy relationships," The Michigan Chapter of the North American Catalysis Society (Virtual) 01/2022
8. "The pursuit of free energies and free energy relationships," Department Seminar, Chemical and Biomolecular Engineering, University of California at Berkeley 12/2021
9. "Dynamical evolution of atomically dispersed catalysts," Pacific Coast Catalysis Society Meeting (Virtual) 10/2021
10. "The pursuit of free energies and free energy relationships," Department Seminar, Chemical Engineering, University of Virginia 09/2021
11. "The pursuit of free energies and free energy relationships," Department Seminar, Chemical Physics, California Institute of Technology (Virtual) 06/2021
12. "The pursuit of free energies and free energy relationships," Truhlar group meeting, Chemistry, University of Minnesota (Virtual) 04/2021
13. "The pursuit of free energies and free energy relationships," Department Seminar, Chemistry and Biochemistry, University of California, San Diego (Virtual) 02/2021
14. "The pursuit of free energies and free energy relationships," Department Seminar, Chemistry and Biochemistry, University of California, Los Angeles (Virtual) 02/2021
15. "Dynamical evolution of atomically dispersed catalysts," Schneider group meeting, Chemical and Biomolecular Engineering, University of Notre Dame (Virtual) 01/2021
16. "The pursuit of free energies and free energy relationships," Department Seminar, Chemical and Environmental Engineering, University of California, Riverside (Virtual) 12/2020
17. "The pursuit of free energies and free energy relationships," Department Seminar, Chemical Engineering, University of California, Davis (Virtual) 12/2020
18. "Metal-free, light-assisted CO_2 reduction: Computational exploration of electron transfer," Claremont Colleges Chemistry Seminar Series (Virtual) 10/2020
19. "Adapting signal recovery algorithms for accurate and efficient reaction rate calculations," Seminar, Mathematics and Computer Science, Argonne National Lab (Virtual) 10/2020
20. "The pursuit of free energies and free energy relationships," Department Seminar, Chemistry, University of California, Merced (Virtual) 10/2020
21. "The pursuit of free energies and free energy relationships," Catalysis Seminar Series, University of California, Santa Barbara (Virtual) 07/2020
22. "Computational tools for catalysis," Department Seminar, Chemical Engineering, Indian Institute of Technology, Bombay 11/2016
23. "Computational tools for catalysis," Department Seminar, Chemical Engineering, Indian Institute of Science, Bangalore 11/2016
24. "Hessian-free methods for catalysis and quantum chemistry," Seminar, Applied Mathematics Department, Lawrence Berkeley National Lab 05/2015
25. "Hessian-free methods for catalysis and quantum chemistry," Seminar, Quantum Simulations Group, Lawrence Livermore National Lab 05/2015

Invited conference talks

26. "Dynamical evolution of atomically dispersed catalysts," Humphrey, N.*, Bac, S.*, **Mallikarjun Sharada, S.** AIChE National Meeting, Phoenix AZ (*upcoming*) 11/2022
27. "Developing design rules for molecular catalysts," Lan, Z.*, Toney, J.*, Kron, K. J.*, Rodriguez-Katakura, A.*, Reed, M.*, Regu, P.*, Elhessen, R.*, **Mallikarjun Sharada, S.** Catalysis and Modeling Symposium, Jens Nørskov's 70th Birthday, Rungsted, Denmark 09/2022
28. "Matrix completion algorithms for efficient calculation of quantum & variational effects in reactions," Quiton, S. J.*, Bac, S.*, Kron, K. J.*, Chae, J., Mitra, U., **Mallikarjun Sharada, S.** World Association of Theoretical and Computational Chemists (WATOC) Congress, Vancouver, Canada 07/2022
29. "Catalyst discovery for metal-free, photoredox CO_2 reduction," Kron, K. J.*, Rodriguez-Katakura, A.*, Reed, M.*, Regu, P.*, Elhessen, R.*, Hunt, J. R., Dawlaty, J., **Mallikarjun Sharada, S.** Molecular Quantum Mechanics Conference, MQM2022, Blacksburg VA 06/2022
30. "Beyond conventional transition state theory in catalysis: Applications of matrix completion methods," Quiton, S. J.*, Bac, S.*, Kron, K. J.*, Chae, J., Mitra, U., **Mallikarjun Sharada, S.** ENFL Symposium, ACS National Meeting, Atlanta GA (Virtual) 08/2021
31. "Incorporating complexity into in silico catalyst design," Lan, Z.*, Humphrey, N.*, Bac, S.*, Quiton, S. J.*, **Mallikarjun Sharada, S.** Telluride Workshop on Exploring Nitrogen Activation Mechanisms (Virtual) 06/2021
32. "Dynamical evolution of atomically dispersed catalysts," Humphrey, N.*, Bac, S.*, **Mallikarjun Sharada, S.** ACS National Meeting (Virtual) 04/2021
33. "Adapting signal recovery algorithms for accurate reaction rate calculations," Quiton, S. J.*, Mitra, U., **Mallikarjun Sharada, S.** Penn Conference in Theoretical Chemistry, Philadelphia PA (Meeting cancelled) 08/2020
34. "Taft equation in inorganic chemistry: Linear free energy relationships for C1 activation," Lan, Z.*, **Mallikarjun Sharada, S.** CATL Symposium, ACS National Meeting, Philadelphia PA (Meeting cancelled) 03/2020
35. "Addressing limitations of density functional theory for transition metal chemistry," Lan, Z.*, **Mallikarjun Sharada, S.** COMP Symposium, ACS National Meeting, San Diego CA. 08/2019
36. "Quantum chemistry," **Mallikarjun Sharada, S.** Discussion leader, Gordon Conference in Computational Chemistry, Mt. Snow VT 07/2018
37. "Conceptual DFT for activity prediction in bio-inspired complexes," Lan, Z.*, **Mallikarjun Sharada, S.** Third Annual Southern California Theoretical Chemistry Conference, Pasadena CA 06/2018
38. "Computational tools for zeolite kinetics: Application to alkane conversion chemistry," **Mallikarjun Sharada, S.**, Bell, A. T., Head-Gordon, M. Gordon Research Seminar, Nanoporous Materials and their Applications, Holderness NH 08/2013

Workshops

39. "Hessian-free methods for stationary point search and characterization: Applications in catalysis," Q-Chem Workshop, Berkeley CA 08/2014

CONTRACTS AND GRANTS

Total external funding: $2.89 M; Sharada's share: $1.51 M
External

1. National Science Foundation (co-PI)
   Title: "CAS: Mild Methods for the Selective De(hydro)chlorination of Polyvinyl Chloride"
   Total Grant Amount: $539,543 (Sharada's share: $159,605)
   Period of Performance: 10/01/2022-09/30/2025
   PI: Megan Fieser (USC), co-PI: Shaama Sharada
2. National Science Foundation (single PI)
   Title: "CAS: Photocatalysis Without Metals - Design Rules for Organic Photoredox Chemistry"
   Total Grant Amount: $306,214

Period of Performance: 09/01/2021 – 08/31/2024
PI: Shaama Sharada

3. Department of Energy Basic Energy Sciences (co-PI)
   Title: "Novel Toolkit for Harnessing the Power of Exascale Computing for Catalyst Design"
   Total Grant Amount: $1,200,000 (Sharada's share: $600,000)
   Period of Performance: 09/01/2021 – 08/31/2025
   PI: Anna Krylov (USC), co-PI: Shaama Sharada
4. Scialog, Research Corporation for Scientific Advancement (PI)
   Title: "Electrifying humidity-swing adsorption for DAC by modulation of redox-polymer hydration"
   Total Grant Amount: $165,000 (Sharada's share: $55,000)
   Period of Performance: 02/15/2021 – 2/14/2023
   PIs: Xiao Su (UIUC), Burcu Gurkan (Case Western Reserve), Shaama Sharada
5. Department of Energy Basic Energy Sciences (PI)
   Title: "Adapting signal recovery algorithms for accurate and efficient reaction rate calculations"
   Total Grant Amount: $571,852 (Sharada's share: $283,122)
   Period of Performance: 09/01/2020 – 08/31/2023
   PI: Shaama Sharada, co-PI: Urbashi Mitra (USC)
6. Doctoral New Investigator, ACS Petroleum Research Foundation (single PI)
   Title: "Atomically dispersed catalysts for direct conversion"
   Total Grant Amount: $110,000
   Period of Performance: 09/01/2020 – 08/31/2023
   PI: Shaama Sharada

Computing grants
Total: $42,303

7. Department of Energy, NERSC Award (co-PI)
   Title "Novel Toolkit for Harnessing the Power of Exascale Computing for Catalyst Design"
   Total Grant Equivalent: - (4,800 Node-Hours)
   Period of Performance: 01/19/2022-01/17/2023
   PI: Anna Krylov (USC), co-PI: Shaama Sharada
8. National Science Foundation, XSEDE Award (single PI)
   Title: "Dynamical evolution of atomically dispersed catalysts"
   Total Grant Equivalent: $11,245 (2,550,000 Service Units)
   Period of Performance: 01/01/2022 – 12/31/2022
9. Department of Energy, NERSC Award (single PI)
   Title: "Adapting signal recovery algorithms for accurate and efficient reaction rate calculations "
   Total Grant Equivalent: - (100,000 Core-Hours)
   Period of Performance: 01/01/2021 – 12/31/2021
10. National Science Foundation, XSEDE Award (single PI)
    Title: "Active site dynamics in atomically dispersed catalysts"
    Total Grant Equivalent: $12,357 (2,321,680 Service Units)
    Period of Performance: 01/01/2021 – 12/31/2021
11. National Science Foundation, XSEDE Award (single PI)
    Title: "Active site dynamics in atomically dispersed catalysts"
    Total Grant Equivalent: $18,701 (1,234,634 Service Units)
    Period of Performance: 07/01/2019 – 06/30/2020

Internal

12. ECET 2022 Chevron Seed Fund (PI)
    Title: "In Silico Catalyst Design Rules for Efficient Gas-to-liquid Conversion"
    Total Amount: $50,000
    Period of Performance: 08/15/2022 – 08/14/2023
    PI: Shaama Sharada, co-PI: Travis Williams
13. Undergraduate Research Associates Program (PI)
    Title: "Exploring green photoredox routes for CO_2 reduction"

Total Amount: $2,000
Period of Performance: 07/01/2021 – 06/30/2022
PI: Shaama Sharada

14. USC Provost New Strategic Directions for Research Award (co-PI)
Title: "Sustainable Production of Fuels and Chemicals using Novel Sulfide Catalysts"
Total Amount: $119,000 (Sharada's share = $29,750)
Period of Performance: 08/01/2020 – 07/31/2021
PI: Jayakanth Ravichandran, co-PIs: Sri Narayan, Brent Melot, Shaama Sharada
15. Zumberge Fund Individual Grant Program (PI)
Total Grant Amount: $30,000
Title: "Catalyst design at the single-atom limit for a hydrogen economy"
Period of Performance: 07/01/2019 – 06/30/2020
PI: Shaama Sharada
16. Undergraduate Research Associates Program (PI)
Title: "Design of enzyme-inspired catalysts for selective and efficient transformation of natural gas"
Total Amount: $2,800
Period of Performance: 07/01/2019 – 06/30/2020
PI: Shaama Sharada

Others: Viterbi Jr Faculty Professional Development Fund ($6,000, 2017-2020); WiSE Supplemental Faculty Support ($7,500, 2017-2020)

CONTRIBUTED CONFERENCE PRESENTATIONS

Students' names are marked with * and presenting author is underlined

1. (Talk) "Dynamic Evolution of Atomically Dispersed Catalysts," Humphrey, N.*, **Mallikarjun Sharada, S.** AIChE National Meeting, Phoenix AZ (*upcoming*) 2022
2. (Talk) "Workflow Automation in Predicting Exciplex Formation in Arene-Amine Complexes," Patra, A.*, **Mallikarjun Sharada, S.** AIChE National Meeting, Phoenix AZ (*upcoming*) 2022
3. (Talk) "Mechanistic Insights into CO Oxidation over Pt1/TiO2: Site-Sensitivity and Dynamic Character of Single Atoms," Bac, S.*, **Mallikarjun Sharada, S.** AIChE National Meeting, Phoenix AZ (*upcoming*) 2022
4. (Talk) "Genetic Algorithm Organic Photoredox Catalyst Evolution for Efficient CO2 Reduction and Degradation Resistance," Kron, K. J.*, **Mallikarjun Sharada, S.** AIChE National Meeting, Phoenix AZ (*upcoming*) 2022
5. (Talk) "Towards Efficient Direct Dynamics Studies of Chemical Reactions: A Novel Matrix Completion Algorithm," Quiton, S. J.*, Bac, S.*, Kron, K. J.*, Chae, J., Mitra, U., **Mallikarjun Sharada, S.** AIChE National Meeting, Phoenix AZ (*upcoming*) 2022
6. (Talk) "Selective Dechlorination Mechanisms with Molecular Catalysts – a Step Towards Polyvinylchloride Upcycling," Bac, S.*, Fieser, M., **Mallikarjun Sharada, S.** AIChE National Meeting, Phoenix AZ (*upcoming*) 2022
7. (Poster) "Genetic Algorithm-Driven Evolution of Organic Photoredox Catalysts for CO_2 Reduction," Kron, K. J.*, **Mallikarjun Sharada, S.** Gordon Research Conference in Catalysis, New London NH 2022
8. (Talk) "Dynamic Evolution of Atomically Dispersed Catalysts," Humphrey, N.*, **Mallikarjun Sharada, S.**, NAM Meeting, New York NY 2022
9. (Talk) "Energy-Efficient CO_2 Reduction with Organic Photoredox Catalysts," Kron, K. J.*, **Mallikarjun Sharada, S.**, NAM Meeting, New York NY 2022
10. (Poster) "CO Oxidation over Atomically Dispersed Pt_1/TiO_2: Atomic-Level Insights into Reaction Pathways and Site-Sensitivity," Bac, S.*, **Mallikarjun Sharada, S.**, NAM Meeting, New York NY 2022
11. (Talk) "Developing Design Rules for Homogeneous Catalysts," Lan, Z.*, **Mallikarjun Sharada, S.**, NAM Meeting, New York NY 2022

12. (Poster) "Beyond Conventional Transition State Theory in Catalysis: Applications of Matrix Completion Methods," Quiton, S. J.*, Bac, S.*, Kron, K. J.*, Chae, J., Mitra, U., **Mallikarjun Sharada, S.**, NAM Meeting, New York NY 2022
13. (Talk) "Framework for developing linear free energy relationships for transition metal complex catalysts," Lan, Z.*, **Mallikarjun Sharada, S.**, ACS Spring Meeting, San Diego CA 2022
14. (Talk, travel award) "Dynamic evolution of atomically dispersed catalysts," Humphrey, N.*, Bac, S.*, **Mallikarjun Sharada, S.**, ACS Spring Meeting, San Diego CA 2022
15. (Talk) "Site sensitivity of Mars-van Krevelen mechanism in CO oxidation over atomically dispersed Pt/TiO_2 catalyst," Bac, S.*, **Mallikarjun Sharada, S.**, ACS Spring Meeting, San Diego CA 2022
16. (Talk) "Beyond conventional transition state theory in catalysis: Applications of matrix completion methods," Quiton, S. J.*, Bac, S.*, Kron, K. J.*, Chae, J., Mitra, U., **Mallikarjun Sharada, S.**, ACS Spring Meeting, San Diego CA 2022
17. (Talk) "An analysis of preferred mechanisms of CO oxidation in TiO_2-supported atomically dispersed catalysts using the energetic span model," Bac, S.*, Humphrey, N.*, **Mallikarjun Sharada, S.**, AIChE National Meeting, Boston MA 2021
18. (Talk) "Dynamical evolution of atomically dispersed catalysts: An ab initio molecular dynamics analysis of thermal and adsorbate-induced metal atom migration," Humphrey, N.*, Bac, S.*, **Mallikarjun Sharada, S.**, AIChE National Meeting, Boston MA 2021
19. (Poster, Award) "Modeling organic photoredox catalyst reduction kinetics, donor-acceptor interactions, and degradation pathways in CO_2 reduction catalytic cycle," Kron, K. J.*, **Mallikarjun Sharada, S.**, AIChE National Meeting, Boston MA 2021
20. (Poster) "Developing linear free energy relationships for transition metal chemistry," Lan, Z.*, **Mallikarjun Sharada, S.**, AIChE National Meeting, Boston MA 2021
21. (Talk) "Beyond conventional transition state theory in catalysis: Applications of matrix completion methods," **Mallikarjun Sharada, S.**, AIChE National Meeting, Boston MA 2021
22. (Poster) "Towards practical matrix completion methods for transition state theory," Quiton, S. J.*, **Mallikarjun Sharada, S.**, AIChE National Meeting, Boston MA 2021
23. (Poster) "An analysis of preferred mechanisms of CO oxidation in atomically dispersed Pt/TiO_2 using the energetic span model," Bac, S.*, **Mallikarjun Sharada, S.**, SUNCAT Summer School (Virtual) 2021
24. (Poster) "Dynamics of atomically dispersed Pt/TiO_2 rutile (110)," Humphrey, N.*, **Mallikarjun Sharada, S.**, SUNCAT Summer School (Virtual) 2021
25. (Poster) "Computational study of organic photoredox catalysts for CO_2 reduction," Kron, K. J.*, **Mallikarjun Sharada, S.**, SUNCAT Summer School (Virtual) 2021
26. (Talk) "Adapting signal recovery algorithms for efficient reaction rate calculations," **Mallikarjun Sharada, S.**, DoE CTC PI Meeting (Virtual) 2021
27. (Talk) "Modeling organic photoredox catalysts for green CO_2 reduction," Kron, K. J.*, **SMS**, ACS Spring Meeting (Virtual) 2021
28. (Talk) "Linear free energy relationships for molecular catalysts: Promise or pipe dream?" Lan, Z.*, **Mallikarjun Sharada, S.**, AIChE National Meeting (Virtual) 2020
29. (Talk) "Exploring green photoredox routes for CO_2 reduction," Kron, K. J.*, **Mallikarjun Sharada, S.**, AIChE National Meeting (Virtual) 2020
30. (Talk) "Ab initio molecular dynamics reveals new active sites in atomically dispersed Pt_1/TiO_2 catalysts," Humphrey, N.*, **Mallikarjun Sharada, S.**, AIChE National Meeting (Virtual). 2020
31. (Talk) "Linear free energy relationships for molecular catalysts: Promise or pipe dream?" Lan, Z.*, **Mallikarjun Sharada, S.**, ACS Fall Meeting (Virtual) 2020
32. (Talk) "Exploring green photoredox routes for CO_2 reduction," Kron, K. J.*, **Mallikarjun Sharada, S.**, ACS Fall Meeting (Virtual) 2020
33. (Talk) "Ab initio molecular dynamics reveals new active sites in atomically dispersed Pt_1/TiO_2 catalysts," Humphrey, N.*, **Mallikarjun Sharada, S.**, ACS Fall Meeting (Virtual) 2020
34. (Poster) "Capturing dynamics of atomically dispersed catalysts: A multiscale approach," Humphrey, N.*, **Mallikarjun Sharada, S.**, International Congress in Catalysis (ICC), San Diego CA (cancelled) 2020

35. (Poster) "CO_2 reduction with organic photoredox catalysts: Substituent effects on electron transfer rates & donor-acceptor interactions," Kron, K. J.*, **Mallikarjun Sharada, S.**, ICC, San Diego CA (cancelled) 2020
36. (Poster) "Reviving Hammett and Taft equations for CH Activation chemistry: Mechanism identification & catalyst design," Lan, Z.*, **Mallikarjun Sharada, S.**, ICC, San Diego CA (cancelled) 2020
37. (Talk) "Active site dynamics in atomically dispersed catalysts," Humphrey, N.*, **Mallikarjun Sharada, S.**, ACS National Meeting, Philadelphia PA (cancelled) 2020
38. (Talk) "Exploring green photoredox routes for CO_2 reduction," Kron, K. J.*, **Mallikarjun Sharada, S.**, ACS National Meeting, Philadelphia PA (cancelled) 2020
39. (Talk) "Active site dynamics in atomically dispersed catalysts," Humphrey, N.*; **Mallikarjun Sharada, S.**, AIChE National Meeting, Orlando FL 2019
40. (Poster) "Elucidating reaction pathways through combined insights from experimental and computational Hammett analysis," Lan, Z.*, **Mallikarjun Sharada, S.**, AIChE National Meeting, Orlando FL 2019
41. (Poster) "Ligand effects on the activity of dicopper catalysts in CH activation," Lan, Z.*, **Mallikarjun Sharada, S.**, SUNCAT Summer Institute, Menlo Park CA 2019
42. (Poster) "Ligand effects on the activity of dicopper catalysts in CH activation," Lan, Z.*, **Mallikarjun Sharada, S.**, Pacific Coast Catalysis Society Meeting, Pullman WA 2019
43. (Talk) "Barrier response analysis as a mechanistic probe for CH activation with bio-inspired complexes," Lan, Z.*, **Mallikarjun Sharada, S.**, North American Meeting (NAM), Chicago IL 2019
44. (Talk) "Barrier Response Analysis Framework to Probe CH Activation Mechanisms," Lan, Z.*, **Mallikarjun Sharada, S.**, ACS Spring Meeting, Orlando FL 2019
45. (Poster) "Tuning catalytic activity in bio-inspired dicopper catalysts," **Mallikarjun Sharada, S.**, Gordon Research Conference, Computational Chemistry, Mt. Snow VT 2018
46. (Poster) "Design principles for atomically dispersed catalysts," **Mallikarjun Sharada, S.**, Air Force Office of Scientific Research Program Review, Albuquerque NM 2018
47. (Talk) "Mechanistic approach to probe ligand-dependence of CH activation kinetics in bioinspired dicopper complexes," **Mallikarjun Sharada, S.**, ACS Spring Meeting, New Orleans LA 2018
48. (Talk) "The surprising accuracy of dispersion-corrected GGAs in prediction of dissociation barriers on transition metal surfaces," **Mallikarjun Sharada, S.**, Bligaard, T., Nørskov, J. AIChE Annual Meeting, Minneapolis MN 2017
49. (Poster) "Peer review in the classroom," **Mallikarjun Sharada, S.**, ASEE Summer School, Raleigh NC 2017
50. (Talk) "Development of Bayesian error estimation density functionals with range-separated exchange," **Mallikarjun Sharada, S.**, Voss, J., Bligaard, T. AIChE Annual Meeting, San Francisco CA 2016
51. (Talk) "Computational examination of the role of the extended framework in alkane conversion in zeolites," **Mallikarjun Sharada, S.**, Bell A. T., Head-Gordon, M. NAM Meeting, Pittsburgh PA 2015
52. (Poster) "Size-independent, hessian-free technique for stationary point search & characterization on potential energy surfaces," **Mallikarjun Sharada, S.**, Bell, A. T., Head-Gordon, M. ACS Fall Meeting, San Francisco CA 2014
53. (Poster) "Computational tools for catalysis: Understanding activity in acidic zeolites," **Mallikarjun Sharada, S.**, Bell, A. T., Head-Gordon, M., GRC, Computational chemistry, Mt. Snow VT 2014
54. (Talk) "QM/MM investigation of the kinetics of cracking and dehydrogenation of n-butane in H-MFI," **Mallikarjun Sharada, S.**, Bell, A. T., Head-Gordon, M. NAM Meeting, Louisville KY 2013
55. (Talk) "Transition state search without exact hessian evaluation," **Mallikarjun Sharada, S.**, Bell, A. T., Head-Gordon, M. ACS Spring Meeting, New Orleans LA 2013
56. (Talk) "Kinetics of alkane cracking & dehydrogenation in H-MFI: Mechanisms & influence of site location," **Mallikarjun Sharada, S.**, Bell, A. T., Head-Gordon, M., Pacific Coast Catalysis Society Meeting, Santa Barbara CA 2012

STUDENT SUPERVISIONS, MENTORING & ADVISING

Current

Postdocs

1. Abhilash Patra (ChemE) (Spr 2022 – present)

Ph.D. Students

1. Kareesa J Kron (ChemE) (Fall 2018 – present)
   Screening Exam: Spring 2019; Qualifying Exam: Spring 2021
2. Nicholas Humphrey (MASC) (Fall 2018 – present)
   Screening Exam: Spring 2019; Qualifying Exam: Spring 2022
3. Selin Bac (ChemE) (Fall 2019 – present)
   Screening Exam: Spring 2020; Qualifying Exam: Summer 2022
4. Kaustubh Rane (ChemE) (Fall 2022 – present)
5. Usama Saleem (ChemE) (Fall 2022 – present)

Undergraduate Students (all ChemE)

1. Sophia Kassabian (Fall 2021 – present)
2. Rachelle Elhessen (Fall 2020 – present)

Graduated students	First job after graduation

PhD Student

Zhenzhuo Lan (ChemE Ph.D. 2022, Defended: 04/18/2022) — Research Scientist, Meta (Facebook)
Dissertation Title: "Linear free energy relationships for transition metal chemistry: Case study of CH activation."

MS Students

1. Pranesh Regu (ChemE, 2019-2020) — Scientist, Alexion Pharmaceuticals
2. Tanya Bansal (ChemE, 2017-2018) — Process Engineer, Repligen Corporation

Undergraduates

1. Stephen Jon Quiton (ChemE, 2018-2022) — PhD student, UC Berkeley
2. Jacob Toney (ChemE, 2018-2021) — Operations engineer, SpaceX (PhD student from Fall 2022, MIT)
3. Miranda Jernberg (ChemE, 2017-2019) — Analyst, BlackRock
4. Joseph Blazer (Physics, 2017-2018) — MS, USC

Other Past Members	Current position

MS Students

1. Bipeng Wang (ChemE, 2018-2020) — PhD student, USC Chemistry
2. Yujia Zhang (ChemE, 2019) — Project Assistant at Laboratory of Neuro Imaging
3. Yichen Gong (ChemE, 2019)

Undergraduates

1. Nicole Nakamoto (ChemE, 2022) — Undergraduate, USC
2. Noah Kim (ChemE, 2022) — Undergraduate, USC
3. Alicia Tsung (ChemE, 2021-2022) — Undergraduate, USC
4. Maria Reed (ChemE, 2021-2022) — Undergraduate, USC (US Navy Officer from 2023)
5. Andres Rodriguez-Katakura (ChemE, 2021-2022) — Undergraduate, USC
6. Mitchell Bias (ChemE, 2019-2020) — Undergraduate, USC
7. Ryan Alimento (ChemE, 2021-2022) — Undergraduate, USC

Visiting Students

1. Vijey Srivathsan (Summer 2019) — MS, USC
2. Allyson Karmazyn (Summer 2019) — PhD, Vanderbilt University

High School Students

1. Sophia Jones, SHINE Program (2022) — Oakwood School
2. Chloe Andrieux-Amadei, SHINE Program (2022) — Windward School
3. Justine Ludden, SHINE Program (2021) — Windward School
4. April Ramos, Young Research Program (2021) — Francisco Bravo Medical Magnet High School
5. Benjamin Barboza, Viterbi Summer Institute (2019) — Undergraduate, USC
6. Cameron Cole, Viterbi Summer Institute (2019) — Undergraduate, USC
7. Samantha Gomez, Young Research Program (2019) — Undergraduate, Santa Monica College
8. Ruoshan Dong, SHINE Program (2018) — Undergraduate, UC Berkeley

Teachers

Ms. Meredith Thomas, Environmental Sciences, Hawthorne Math and Science Academy (2020)

STUDENT AWARDS AND HONORS

1. Kareesa Kron (PhD, current)
   a. USC WiSE Travel Award, 2022
   b. Kokes Award, 27th North American Catalysis Society Meeting (NAM27), 2022
   c. Special Mentions (Oral Presentation), MFD Student Symposium, 2022
   d. AIChE Catalysis and Reaction Engineering Best Poster Award, 2021
   e. TLARGI Fellowship, MFD, 2021
   f. Invitee, ACS Green Chem Summer School, 2021
   g. International Congress in Catalysis Travel Award, 2020
   h. Mork Fellowship, MFD, 2019
   i. Graduate Poster Award, MFD Student Symposium, 2019
   j. NSF Graduate Research Fellowship Program (GRFP) Special Mention, 2019
   k. One-year graduate fellowship, USC, 2018

2. Nicholas Humphrey (PhD, current)
   a. ACS Spring Meeting CATL-ChemCatBio Graduate Student Travel Award, 2022
   b. NSF GRFP Special Mention, 2019
   c. One-year graduate fellowship, USC, 2018

3. Selin Bac (PhD, current)
   a. Graduate Poster Award, MFD Student Symposium, 2022
   b. One-year graduate fellowship, USC, 2018

4. Usama Saleem (PhD, current)
   a. One-year graduate fellowship, USC, 2022

5. Zhenzhuo Lan (PhD, former)
   a. TLARGI Fellowship, MFD, 2020
   b. WiSE Travel Award, USC, 2019
   c. Two-year graduate fellowship, USC, 2017

6. Rachelle Elhessen (Undergraduate, current)
   a. WiSE Aerospace Corporation Research Fellowship, 2021

7. Stephen Quiton (Undergraduate, former)
   a. Awardee, NSF GRFP, 2022
   b. USC Discovery Scholar, 2022
   c. USC Viterbi Best Research Paper Award, 2022
   d. USC Viterbi Albert Dorman Scholar Award, 2022
   e. USC Viterbi Charles J. Rebert Chemical Engineering Outstanding Student Award, 2022
   f. Second Prize, USC Viterbi Undergraduate Symposium, 2022
   g. Undergraduate Poster Award, USC MFD Student Symposium, 2022
   h. USC Dornsife Student Opportunities for Academic Research (SOAR) Fellowship, Spring 2022
   i. USC Provost Undergraduate Research Fellowship, Spring 2021, Fall 2020

j. MFD Symposium Undergraduate Poster Award, 2021
k. Barry Goldwater Scholarship, 2020
l. Best Poster, AIChE Annual Student Conference, Computing and Process Control, 2020
m. First Prize, AIChE Western Regional Conference, Technical Presentation Competition, 2020
n. USC Finalist, Astronaut Foundation Scholarship, 2020
o. USC Viterbi Engineering Associates Award, 2019

7. Jacob Toney (Undergraduate, former)
   a. University Trustees Award, USC, 2021
   b. USC Viterbi Albert Dorman Valedictorian Scholar Award, 2021
   c. USC Viterbi Best Research Paper, 2021
   d. USC Viterbi Charles J. Rebert Chemical Engineering Outstanding Student Award, 2021
   e. MFD Symposium Undergraduate Oral Presentation Award, 2021
   f. USC Provost Undergraduate Research Fellowship, Fall 2020, Spring 2020, Spring 2019
   g. USC Presidential Scholarship, 2017

TEACHING

- Spring 2018 – CHE 544: Graduate Heat Transfer (also DEN)
  Enrollment: 26 Contact hours: 3
- Fall 2018 – CHE 450: Sustainable Energy
  Enrollment: 14 Contact hours: 3
- Spring 2019 – CHE 544: Graduate Heat Transfer (also DEN)
  Enrollment: 37 Contact hours: 3
- Fall 2019 – CHE 450: Sustainable Energy
  Enrollment: 18 Contact hours: 4
- Spring 2020 – CHE 544: Graduate Heat Transfer (also DEN)
  Enrollment: 23 Contact hours: 3
- Fall 2020 – CHE 450: Sustainable Energy
  Enrollment: 12 Contact hours: 4
- Spring 2021 – CHE 350: Introduction to Separation Processes
  Enrollment: 39 Contact hours: 4
- Fall 2022 – CHE 450: Sustainable Energy
  Enrollment: 14 Contact hours: 4
- Spring 2022 – CHE 350: Introduction to Separation Processes
  Enrollment: 43 Contact hours: 4

MEMBERSHIP

1. ACS – American Chemical Society (2018 – present)
2. AIChE – American Institute of Chemical Engineers (2016 – present)

SERVICE

External

Program Chair
ACS Catalysis Division, Fall National Meeting (*upcoming*) 2023, 2024
Conference Organization
1. Abstract reviewer, North American Catalysis Society Meeting 2022, 2019
2. Poster judge, 10th Triennial Conference on Molecular Quantum Mechanics 2022
3. Abstract reviewer, International Congress in Catalysis 2020
4. Local Arrangements Committee, International Congress in Catalysis 2020
5. Lead organizer, Fourth Annual Southern California Theoretical Chemistry Conference 2019

Conference Session Chair
1. Complexity in Computational Catalysis, ACS Spring Meeting 2022, 2021
2. Catalysis and Reaction Engineering Poster Session, AIChE National Meeting 2021, 2022

3. Chair/Co-Chair, New Developments in Computational Catalysis, AIChE National Meeting 2020, 2019, 2018, 2017
4. Discussion leader, Gordon Research Conference, Computational Chemistry 2018
5. Discussion leader, Gordon Research Seminar, Computational Chemistry 2014

Reviewer

Grant Agencies

1. National Science Foundation (2 panels) 2018-Present
2. Department of Energy (~ 1 grant/year) 2018-Present
3. American Chemical Society Petroleum Research Fund (~ 1 grant/year) 2019-Present

Journals

ACS Catalysis, Chemical Engineering Science, Chemical Physics Letters, Journal of the American Chemical Society, Journal of Catalysis, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Journal of Organic Chemistry, Journal of Physical Chemistry Letters, Molecular Physics, Nature Communications, Physical Chemistry Chemical Physics, PNAS Nexus, Scientific Reports, Surface Science

Internal

University

- Proposal reviewer, Office of Research 2021
- Founding Faculty Advisor, Women in Chemical Engineering (WChE). 2019-present

School

- Collaborate with USC STEM Center to conduct webinars and host teachers from Hawthorne Math and Science Academy in summer to incorporate modeling and visualization software in high school classrooms 2020-present
- "Make a molecule" webinar for Viterbi K-12 STEM outreach 2020
- Guest Speaker, USC Viterbi SHINE Program 2018

Department

- Member, Faculty Search Committee (Tenure-track Assistant Professor) 2021-2022
- Chair, MFD Student Research Symposium Committee 2018-2022
- Chair, Graduate visiting weekend 2018-2020
- Member, Graduate Recruitment Committee 2018-2020

Exam Committees

Screening Exam

- 2017: Fang Fu (Chemistry)
- 2018: Ariel Nessl (Chemistry), Anyue Jiang (Petroleum), Bryan Nguyen (ChemE), Fatemeh Sadat Zebarjad (ChemE)
- 2019: Belinda Garana (ChemE), Kylie Trettner (ChemE)
- 2020: Sourav Dey (Chemistry), Stacey Bacheller (ChemE), Linghao Zhao (ChemE), Razieh Etezadi (ChemE)
- 2021: Ziyue Zhu (Chemistry)

Qualifying Exam

- 2017: Jitendra Gurjar (Chemistry), Fang Fu (Chemistry)
- 2018: Subodh Tiwari (MASC), Ariel Nessl (Chemistry), Christine Cheng (ChemE), Nareh Movsesian (ChemE)
- 2019: Fatemeh Sadat Zebarjad (ChemE)
- 2020: Jung Hwan Shin (MASC), Roya Ermagan (ChemE)
- 2021: Melanie MacMullan (ChemE), Sourav Dey (Chemistry), Suyue Yuan (MASC)
- 2022: Boyang Zhao (MASC), Stacey Bacheller (ChemE), Majed Madani (ChemE), Ziyue Zhu (Chemistry), Anikeya Aditya (MASC), Bin Pan (ChemE), Razieh Etezadi (ChemE)

Thesis Defense

- 2019: Ivan Demianets (Chemistry)
- 2020: Jitendra Gurjar (Chemistry)
- 2021: Fang Fu (Chemistry), Jung Hwan Shin (MASC), Fatemeh Sadat Zebarjad (ChemE)
- 2022: Billal Zayat (Chemistry)