Shaama Mallikarjun Sharada

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Mork Family Department of Chemical Engineering & Materials Science, VHE 516, University of Southern California, Los Angeles 900089, USA
ssharada@usc.edu
http://sharada-lab.usc.edu

Education and Qualifications

Aug 2015	Ph.D., Chemical Engineering Minor: Physical Chemistry	University of California at Berkeley
Aug 2008	B.Tech, M.Tech, Chemical Engineering Process Systems Design and Engineering	Indian Institute of Technology, Bombay

Positions

2017–Present	**WiSE Gabilan Assistant Professor**, University of Southern California
2015–2017	**Postdoctoral Researcher**, Chemical Engineering, Stanford University
2011–2015	**Developer**, Q-Chem Inc., *ab initio* quantum chemistry software
2008–2010	**Business Analyst**, A. T. Kearney India Ltd., Management consulting
Spring 2008	**Visiting Scientist**, Max Planck Institute, Magdeburg, Germany
Summer 2006	**Young Engineering Fellow**, Indian Institute of Science, Bangalore, India

Honors and Awards

2017	WiSE Gabilan Jr. Chair, University of Southern California
2015	Kokes Award, 24th North American Catalysis Society
2014	Invitee, 128th International Summer Course, BASF, Ludwigshafen
2008	Institute Gold Medal & Institute Silver Medal, Indian Institute of Technology, Bombay
2006	Young Engineering Fellowship, Indian Institute of Science, Bangalore
2006	IIT Bombay Heritage Fund Scholarship

Grants

Internal USC Awards

2019-20	$30,000	Zumberge Fund Individual Grant Program
2019-20	$2,800	Undergraduate Research Associates Program
2018-19	$2,500	WiSE Supplemental Faculty Support
2018-19	$2,000	Viterbi Jr Faculty Professional Development Fund
2017-18	$2,000	Viterbi Jr Faculty Professional Development Fund
2017-18	$2,500	WiSE Supplemental Faculty Support

Invited Talks

2018	'Conceptual DFT for activity prediction in bio-inspired complexes,' Third Annual Southern California Theoretical Chemistry Conference, Pasadena CA
2016	'Computational tools for catalysis,' Department of Chemical Engineering, Indian Institute of Technology, Bombay, Mumbai, India
2016	'Computational tools for catalysis,' Department of Chemical Engineering, Indian Institute of Science, Bangalore, India
2015	'Hessian-free methods for catalysis and quantum chemistry,' Applied Mathematics Department, Lawrence Berkeley National Lab, Berkeley CA
2015	'Hessian-free methods for catalysis and quantum chemistry,' Quantum Simulations Group, Lawrence Livermore National Lab, Livermore CA
2014	'Hessian-free methods for stationary point search and characterization: Applications in catalysis,' Q-Chem Workshop, Berkeley CA
2013	'Computational tools for zeolite kinetics: application to alkane conversion chemistry,' Gordon Research Seminar, Nanoporous materials & their applications, Holderness NH

Conference Presentations

2019 'Barrier Response Analysis Framework to Probe CH Activation Mechanisms,'
Talk, ACS National Meeting, Orlando FL

2018 'Tuning catalytic activity in bio-inspired dicopper catalysts,'
Poster, Gordon Research Conference, Computational chemistry, Mt. Snow VT

2018 'Design principles for atomically dispersed catalysts,'
Poster, AFOSR Molecular Dynamics/Theoretical Chemistry Program Review, Albuquerque, NM

2018 'Mechanistic approach to probe ligand-dependence of CH activation kinetics in bioinspired dicopper complexes,'
Talk, ACS National Meeting, New Orleans LA

2017 'The surprising accuracy of dispersion-corrected GGAs in prediction of dissociation barriers on transition metal surfaces,'
Talk, AIChE Annual Meeting, Minneapolis MN

2017 'Peer review in the classroom,'
Poster, ASEE Summer School, Raleigh NC

2016 'Development of Bayesian error estimation density functionals with range-separated exchange,'
Talk, AIChE Annual Meeting, San Francisco CA

2015 'Computational examination of the role of the extended framework in alkane conversion in zeolites,'
Talk, 24th NAM, North American Catalysis Society, Pittsburgh PA

2014 'Size-independent, hessian-free technique for stationary point search & characterization on potential energy surfaces,'
Poster, 248th ACS National Meeting, San Francisco CA

2014 'Computational tools for catalysis: Understanding activity in acidic zeolites,'
Poster, Gordon Research Seminar & Conference, Computational chemistry, Mt. Snow VT

2013 'QM/MM investigation of the kinetics of cracking and dehydrogenation of n-butane in H-MFI,'
Talk, 23rd NAM, North American Catalysis Society, Louisville KY

2013 'Transition state search without exact hessian evaluation,'
Talk, 245th ACS National Meeting, New Orleans LA

2012 'Kinetics of alkane cracking and dehydrogenation in H-MFI: Mechanisms & influence of acid site location,'
Talk, Pacific Coast Catalysis Society Annual Meeting, Santa Barbara CA

Publications

1. '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. **2018**, *under review*

2. 'Computational Strategies to Probe CH Activation in Dioxo-Dicopper Complexes,'
Lan, Z.; Mallikarjun Sharada, S. **2018 PCCP HOT Articles**, Physical Chemistry Chemical Physics, **2018**, 20, 25602-25614.

3. '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.

4. '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.

5. 'Theoretical analysis of the influence of pore geometry on monomolecular cracking and dehydrogenation of n-butane in Brønsted-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.

6. '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. **Special Issue**, Molecular Physics, **2015**, 113, 1802-1808.

7. '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.

8. '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.
9. '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.
10. 'Advances in molecular quantum chemistry contained in the Q-Chem 4 program package,' Shao, Y.; Gan Z.; Epifanovsky, E.; ...; Mallikarjun Sharada, S. et al. Molecular Physics, **2015**, 113, 184-215.
11. '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.
12. '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.
13. 'Automated transition state searches without evaluating the hessian,'
Mallikarjun Sharada, S.; Zimmerman, P. M.; Bell, A. T.; Head-Gordon, M. **Special Issue**, Journal of Chemical Theory and Computation, **2012**, 8, 5166-5174.
14. '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.
15. '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.

Teaching

2018	**Instructor**, CHE450: Sustainable Energy
2018-19	**Instructor**, CHE544: Graduate heat transmission
2016	**Teaching assistant**, ChemEngg-444: Electronic structure theory, applications to chemical kinetics
2013	**Teaching assistant**, CBE-162: Chemical engineering process control
2011	**Teaching assistant**, CBE-154: Chemical engineering lab
2007	**Teaching assistant**, CL-431: Chemical engineering lab

Mentoring

Graduate Students

2017–Present	Zhenzhuo Lan, Ph.D., 2-year Graduate Fellowship recipient (2017)
2018–Present	Kareesa Kron, Ph.D., 1-year Graduate Fellowship recipient (2018)
2018–Present	Nicholas Humphrey, Ph.D., 1-year Graduate Fellowship recipient (2018)
2019–Present	Yujia Zhang, Masters
2019–Present	Yichen Gong, Masters
2018–Present	Bipeng Wang, Masters
2017–2018	Sathvika Seshasayee Lnu, Masters
2017–2018	Tanyarajeev Bansal, Masters
2015–17	Linan Zhang, Ph.D.

Undergraduate Students

2018–Present	Jacob Toney, Provost's Fellowship recipient (2019)
2018–Present	Stephen Quiton
2017–Present	Miranda Jernberg
2017–2018	Joseph Blazer

High School Students

2018 Summer	Ruoshan Dong

Professional Service

2019-2020	**Organizing Committee, Local Arrangements**, International Congress in Catalysis 2020
2019	**Session Co-Chair**, 'New developments in computational catalysis,' AIChE Annual Meeting
2019	**Co-Organizer**, Fourth Annual Southern California Theoretical Chemistry Conference
2019	**Abstract reviewer**, 2019 North American Catalysis Society Meeting (NAM26)
2018	**Discussion leader**, Gordon Research Conference, Computational Chemistry
2018	**Proposal review panel member**, NSF Directorate for Engineering (ENG)
2018	**Proposal reviewer**, DoE Chemical Sciences, Geosciences, & Biosciences (CSGB) Division
2018	**Session chair**, 'New developments in computational catalysis,' AIChE Annual Meeting
2018–Present	**Member**, American Chemical Society
2017	**Co-chair**, 'New developments in computational catalysis,' AIChE Annual Meeting
2016–Present	**Senior member**, American Institute of Chemical Engineers
2014	**Discussion leader**, Gordon Research Seminar, Computational Chemistry
	Reviewer, Molecular Physics, Chemical Engineering Science, ACS Catalysis, Physical Chemistry Chemical Physics, Scientific Reports, Journal of Physical Chemistry