SHAAMA MALLIKARJUN SHARADA

(510) 316 – 3177 shaama@stanford.edu

EDUCATION

2015 Ph.D. Chemical Engineering
University of California, Berkeley
Dissertation: "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: Alexis T. Bell, Martin Head-Gordon

2008 M.Tech, B.Tech, Chemical Engineering
Indian Institute of Technology, Bombay
Institute Gold Medal for highest GPA (9.51/10) in the graduating class

PROFESSIONAL EXPERIENCE

2015- **Postdoctoral Researcher**
SUNCAT, Stanford University (10/2015 -)
Developing Bayesian Error Estimation Functionals (BEEF) with exact exchange
Advisors: Thomas Bligaard, Jens Nørskov

2015 **Graduate Student Researcher**
University of California, Berkeley (08/2010 – 08/2015)
Developed novel Davidson-based scheme for wavefunction stability analysis
Devised automated method for transition state (TS) search and characterization
Analyzed sensitivity of light alkane activation to zeolite catalyst pore topologies

2015 **Developer**
Q-Chem. Inc., ab initio quantum chemistry software (2011 – 2015)
Implemented codes for TS search, characterization, and stability analysis

2010 **Business Analyst**, Management Consulting
A. T. Kearney India Ltd. (07/2008 – 05/2010)
Retail launch and operation: responsible for global trends, site selection, and merchandise modules in convenience store retail strategy for a large company

2008 **Master's Student**
IIT Bombay; Max Planck Institute, Magdeburg (05/2007 – 06/2008)
Advisors: Sanjay M. Mahajani, Achim Kienle
Simulated reactive chromatography process models for series-parallel reactions

2006 **Young Engineering Fellow**
Indian Institute of Science, Bangalore (05/2006 – 07/2006)
Devised polymer degradation models for combined ultrasonic and UV conditions

PROFESSIONAL SERVICE

2015- Reviewer: Journal of Molecular Physics, Chemical Engineering Science
2014 Discussion Leader: Gordon Research Seminar, Computational Chemistry

SHAAMA MALLIKARJUN SHARADA

(510) 316 – 3177 shaama@stanford.edu

PUBLICATIONS

"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.

"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.

"Analysis of the effects of temperature and n-alkane chain length on thermodynamics of adsorption and on intrinsic activation barriers for monomolecular cracking by Brønsted-acid sites in MFI using CBMC simulations and QM/MM,"
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.

"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.

"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.

"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.

"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.

"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.

"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.

MANUSCRIPTS (in preparation)

"Computational examination of the influence of pore geometry on monomolecular reactions of n-butane in Brønsted-acid Zeolites,"
Mallikarjun Sharada, S.; Janda, A.; Bell, A. T.; Head-Gordon, M.

SHAAMA MALLIKARJUN SHARADA

(510) 316 – 3177 shaama@stanford.edu

INVITED TALKS

2015 "Hessian-free methods for catalysis and quantum chemistry," 07/16/2015
Applied Mathematics Department, Lawrence Berkeley National Lab, Berkeley CA

2015 "Hessian-free methods for catalysis and quantum chemistry," 07/13/2015
Quantum Simulations Group, Lawrence Livermore National Lab, Livermore CA

2014 "Hessian-free methods for stationary point search and characterization: Applications in catalysis," 08/09/2014
Q-Chem Workshop, Berkeley CA

2013 "Computational tools for zeolite-based kinetics: applications to alkane conversion chemistry," 08/11/2013
Gordon Research Seminar, Nanoporous materials & their applications, Holderness NH

CONFERENCE PRESENTATIONS

2015 Talk: "Computational examination of the role of the extended framework in alkane conversion in zeolites," 06/18/2015
24th NAM, North American Catalysis Society, Pittsburgh PA

2014 Poster: "Size-independent, hessian-free technique for stationary point search and characterization on potential energy surfaces," 08/12/2014
248th ACS National Meeting, San Francisco CA

2014 Poster: "Computational tools for catalysis: Understanding activity in acidic zeolites," 07/20/2014
Gordon Research Seminar, Conference, Computational chemistry, Mt. Snow VT

2013 Talk: "QM/MM investigation of the kinetics of cracking and dehydrogenation of n-butane in H-MFI," 06/03/2013
23th NAM, North American Catalysis Society, Louisville KY

2013 Talk: "Transition state search without exact hessian evaluation," 04/07/2013
245th ACS National Meeting, New Orleans LA

2012 Talk: "Kinetics of alkane cracking and dehydrogenation in H-MFI: Mechanisms and influence of acid site location," 09/24/2012
Pacific Coast Catalysis Society Annual Meeting, Santa Barbara CA

AWARDS AND HONORS

2015 Kokes Award, 24th North American Catalysis Society
2014 Invitee, 128th International Summer Course, BASF, Ludwigshafen
2008 Institute Silver Medal, Indian Institute of Technology (IIT), Bombay
2006 IIT Bombay Heritage Fund Scholarship

TEACHING EXPERIENCE

2016 ChemEngg-444: Electronic structure theory, applications to chemical kinetics
2013 CBE-162: Chemical engineering process control
2011 CBE-154: Chemical engineering lab
2007 CL-431: Chemical engineering lab