Ambarish Kulkarni

Department of Chemical Engineering
Stanford University, Stanford, CA 94305
404-408-2324 ambarish@stanford.edu

EDUCATION

Postdoctoral Research 2015 – present
Stanford University, Stanford, CA
Advisor: Jens K. Nørskov

Ph.D. in Chemical Engineering 2009 – 2014
Georgia Institute of Technology, Atlanta, GA
Advisor: David S. Sholl and Christopher W. Jones

B.S. in Chemical Engineering 2005 – 2009
Institute of Chemical Technology (formerly UDCT), Mumbai, India

RESEARCH EXPERIENCE

Postdoctoral Fellow | Jens Nørskov 2015 – present
Stanford University, Stanford, CA

- Identified the active site and reaction mechanism of partial methane activation in various zeolites
- Developed a universal descriptor for predicting C-H bond activation rates in different catalyst classes and screened materials for selective methane oxidation
- Designed and optimized novel metal-organic framework based catalysts for electrochemical CO_2 and O_2 reduction reactions
- *Collaborations:* Matteo Cargnello, Zhenan Bao (Stanford); Yuriy Roman-Leshkov (MIT)

Graduate Student | David Sholl 2009 – 2014
Georgia Institute of Technology, Atlanta, GA

- Screened a large database of metal-organic frameworks (MOFs) and zeolites for industrially relevant gas separations using *ab-inito* derived force fields
- Developed a flexible force field to predict the stability, diffusion properties and dynamics of MOFs from first principles
- Successfully demonstrated the techno-economic feasibility processes for direct capture of CO_2 from air using process simulation methods
- *Collaborations:* Krista Walton, Sankar Nair, Christopher Jones (Georgia Tech)

Research Intern | Preeti Kamakoti Jun – Aug 2013
Corporate Strategic Research, ExxonMobil, NJ

- Developed DFT derived force fields for modeling H_2S and CO_2 adsorption in cationic zeolites
- Implemented a user friendly, molecular modeling based toolkit to accelerate materials discovery for industrial separations

Undergraduate Researcher | Shriniwas Samant 2007 – 2008
Institute of Chemical Technology, Mumbai

- Evaluated novel strategies for synthesis of zeolite catalysts for hydrogenation reactions

RESEARCH PROPOSALS

- **Center for Nanoscale Materials, Argonne National Laboratory** 2016 – 2017
  Screening of cation-exchanged zeolites for direct partial oxidation of methane to methanol. (Allocated 590,000 hours, PI: Ambarish Kulkarni)

- **Center for Nanoscale Materials, Argonne National Laboratory** 2017 – 2018
  Design and screening of metal-organic frameworks for electrochemical CO_2 and O_2 reduction reactions. (Under review, PI: Ambarish Kulkarni)

PUBLICATIONS

(* = co-first author, Total first author publications = 7)

1. Latimer, A. A.*, Kulkarni, A. R.*; Aljama, H.; Yoo, J. S.; Tsai, C.; Abild-Pedersen, F.; Studt, F.; Nørskov, J. K., Understanding Trends in C-H Bond Activation in Heterogeneous Catalysis. *(Nature Mat., in-press, DOI: 10.1038/nmat4760)*
2. Kulkarni, A. R.; Sholl, D. S., Screening of Copper Open Metal Site MOFs for Olefin/Paraffin Separations Using DFT Derived Force Fields *(J. Phys. Chem. C, in-press, DOI: 10.1021/acs.jpcc.6b07493)*
3. Kulkarni, A. R.; Zhao, Z.-J.; Siahrostami, S.; Nørskov, J. K.; Studt, F., Mono-Copper Active Site for Partial Methane Oxidation in Cu-Exchanged 8MR Zeolites. *ACS Catal.*, **2016**, *6*, pp 6531–6536.
4. Zhao, Z.-J.; Kulkarni, A. R.; Vilella, L.; Nørskov, J. K.; Studt, F., Theoretical Insights into the Selective Oxidation of Methane to Methanol in Copper-Exchanged Mordenite. *ACS Catal.*, **2016**, *6* (6), pp 3760–3766.
5. Fang, H.*; Kulkarni , A. R.*; Kamakoti, P.; Awati, R.; Ravikovitch, P. I.; Sholl, D. S., Identification of High CO_2 Capacity Cationic Zeolites by Accurate Computational Screening. *Chem. Mater.*, **2016**, *28* (11), pp 3887–3896.
6. Nie, X.; Kulkarni, A. R.; Sholl, D. S., Computational Prediction of Metal Organic Frameworks Suitable for Molecular Infiltration as a Route to Development of Conductive Materials. *J. Phys. Chem. Lett.*, **2015**, *6* (9), pp 1586–1591.
7. Kulkarni, A. R.; Sholl, D. S., DFT-Derived Force Fields for Modeling Hydrocarbon Adsorption in MIL-47 (V). *Langmuir*, **2015**, *31* (30), pp 8453–8468.
8. Cai, Y.*; Kulkarni , A. R.*; Huang, Y.-G.; Sholl, D. S.; Walton, K. S., Control of MOF Crystal Topology by Ligand Functionalization: Functionalized HKUST-1 Derivatives. *Cryst. Growth Des.*, **2014**, *14* (11), pp 6122–6128.
9. Didas, S. A.; Kulkarni, A. R.; Sholl, D. S.; Jones, C. W., Role of Amine Structure on CO_2 Adsorption from Ultradilute Gas Streams Such as Ambient Air. *ChemSusChem* 2012, *5* (10), pp 2058-2064.
10. Kulkarni, A. R.; Sholl, D. S., Analysis of Equilibrium-Based TSA Processes for Direct Capture of CO_2 from Air. *Ind. Eng. Chem. Res.*, **2012**, *51* (25), pp 8631–8645.

INVITED TALKS

- A.R. Kulkarni, DFT-based Tools for Predicting Adsorption and Screening of Porous Materials, *Corporate Strategic Research, ExxonMobil*, Aug 7 2013.
- A.R. Kulkarni, Applications of Density Functional Theory: Multiscale Modeling of Nanoporous Materials. *Department of Chemistry, University of Minnesota*, Sep 8 2014.

PATENTS

- Fang, H.; Kulkarni, A. R.; Awati, R. V.; Sholl, D. S., Adsorbent Materials and Methods of Adsorbing CO_2, Nov 18 2015, U.S. Serial No 62/255,789.

CONFERENCE PRESENTATIONS

- A. R. Kulkarni, A. A. Latimer, F. Studt, J. K. Nørskov, Screening of Active Site Motifs for C-H Bond Activation in Nanoporous Catalysts, *AICHE Annual Meeting,* San Francisco, 2016.
- A. R. Kulkarni and D. S. Sholl, Screening of Copper Open Metal Site MOFs for Olefin/Paraffin Separations using DFT Derived Force Fields, *AICHE Annual Meeting,* San Francisco, 2016.
- A. R. Kulkarni, J. K. Nørskov and F. Studt**,** Screening of Active Site Motifs for Direct Partial Oxidation of Methane to Methanol, *International Catalysis Congress,* Beijing, China, 2016.
- A. R. Kulkarni, J. K. Nørskov and F. Studt**,** Universal Descriptor based Screening of Active Site Motifs for C-H Bond Activation, *Gordon Research Conference: Catalysis,* New London, 2016. (Poster)
- A. R. Kulkarni, Z-., J. Zhao, J. K. Nørskov and F. Studt**,** Mechanism for Direct Partial Oxidation of Methane to Methanol in 8MR Zeolites, *ACS National Meeting*, San Diego, 2016.
- A.R. Kulkarni, J. Gee and D. S. Sholl, Applications of DFT Derived Force Fields for Olefin/ Paraffin Separation in MOFs, *AICHE Annual Meeting*, Atlanta, 2014.
- A.R. Kulkarni, Y. Cai, K.S. Walton and D. S. Sholl, Experimental and Modeling Studies in CuBTC Metal-Organic Frameworks: Functionalization Induced Polymorphism, *11th International Conference on the Fundamental of Adsorption,* Baltimore, 2013 and *AICHE Annual Meeting*, Pittsburgh, 2012.
- A. R. Kulkarni, S. A. Didas, C. W. Jones, D. S. Sholl, Technological and economic analysis of adsorption processes for capture of CO_2 from air, *AICHE Annual Meeting*, Pittsburgh, 2012.
- A. R. Kulkarni, S. A. Didas, C. W. Jones, D. S. Sholl, Modeling adsorption processes for direct capture of CO_2 from air, *AICHE Annual Meeting*, Minneapolis, 2011 and *17th Symposium on Separation Science and Technology*, Gatlinburg, 2011.

TEACHING EXPERIENCE

Guest Lecturer, Basic Principles of Heterogeneous Catalysis — May 2016
Stanford University, Stanford, CA

- Classroom instruction for graduate students

Teaching Assistant, Electronic Structure Theory and Applications to Kinetics — Jan – April 2016
Stanford University, Stanford, CA

- Guided graduate students in performing hands-on DFT calculations aimed at solving realistic research projects

Teaching Assistant, Chemical Engineering Numerical Methods — Aug – Dec 2012, May – Aug 2011, May – Aug 2010
Georgia Institute of Technology, Atlanta, GA

- Taught classes, graded assignments and held office hours for undergraduate students

National Workshop, Research Experience in Carbon Sequestration — Jun 2011
University of Alabama, Birmingham, AL

- Organized classroom sessions, group exercise and research activities relating to Carbon Capture and Sequestration

MANUSCRIPTS IN-PREPARATION

1. Kulkarni, A. R.; Zhao, Z-. J.; F.; Nørskov, J. K.; Studt, F., Cation-Exchanged Zeolites for the Selective Oxidation of Methane to Methanol.
2. Siahrostami, S.; Kulkarni, A. R.; Studt, F.; Nørskov, J. K., Porous Materials with Single-Metal Active Site: Potential Catalysts for Oxygen Reduction Reaction.
3. Kulkarni, A. R.; Siahrostami, S.; Studt, F.; Nørskov, J. K., Mechanism of CO_2 Reduction in Porphyrin-based MOFs from DFT Calculations.
4. Kulkarni, A. R.; Nørskov, J. K.; Studt, F., Scaling Relations for Adsorption of CH_x and SiH_x Species on Transition Metal Surfaces.
5. Verploegh, R. J.; Kulkarni A. R.; Tang, D.; Boulfelfel, S.; Sholl D. S., A DFT Parameterized Force Field for ZIFs: Application to Gas Diffusion.

SERVICE AND HONORS

- **Peer Reviewer**, Langmuir, Energy and Environ. Sci., J. Phys. Chem. C, ACS Catal.
- **Travel Award,** Gordon Research Conference: Catalysis, New London (2016)
- **Chair,** Media committee, ChBE Graduate Symposium at Georgia Tech (2011)
- **Judge**, President Undergraduate Research Award proposals at Georgia Tech (2010)
- **Fellow**, National Incentive for Undergraduate Research (2008)