Megha Anand

Contact Information

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Research Interests

Computational Chemistry, Heterogeneous and Homogeneous Catalysis, Electrochemistry, Reaction Mechanism, Solvent Effects, Active Learning

Education

University of Georgia Athens, Georgia USA
Center for Computational Quantum Chemistry

Ph.D., Chemistry (August 2012-May 2016)

- Dissertation topic: Theoretical studies on the role of silver salt additives in palladium catalysis
- Advisor: **Henry F. Schaefer III**

Indian Institute of Technology Bombay, Mumbai, India

5-year Integrated M.S. in Chemistry with Minor in Biosciences and Bioengineering (April 2012)

- Dissertation topic: Density functional theory studies on mechanism of transition metal catalysed double C–H activation reactions
- Advisor: **Raghavan B. Sunoj**

Research Experience

Post-doctoral Associate, Technical University of Denmark **Aug 2018 - till now**
Catalysis Theory Center
Advisor: **Jens K. Nørskov**

- Computational study on doped oxides as stable materials for oxygen reduction reaction
- Develop new methods for homogeneous catalysis using data intensive approaches
- *In silico* catalyst discovery for electrochemical oxidation of molecular nitrogen to nitrates
- Active learning to discover molecular catalysts for challenging homogeneous reactions

Post-doctoral Associate, Stanford University, California **Jan 2017 - Jul 2018**
SUNCAT Center for Surface Science and Catalysis
Advisor: **Jens K. Nørskov**

- Computationally studied oxygen reduction reaction on gold-supported metal porphycenes

Graduate Student, University of Georgia Athens, Georgia USA **Aug 2012 - May 2016**
Center for Computational and Quantum Chemistry
Advisor: **Henry F. Schaefer III**

- Studied the molecular level role of silver additives in a palladium catalyzed amination reactions using Density Funtional Theory
- Worked with (late) Prof. Paul Schleyer and Dr. Judy Wu on the hydrogen bond–Aromaticty cooperativity in 4-Pyridone chains

Undergraduate Researcher, IIT Bombay, India **Apr 2008 - Apr 2012**
Computational Chemistry Group
Advisor: **Raghavan B. Sunoj**

- Explored reaction mechanisms and solvent effects on C–H activation reactions
- Complex micro-solvated transition states were identified for reactions in protic solvents

PUBLICATIONS

Anand, M.; Rohr, B.; Statt, M. J.; and Nørskov, J. K. *J. Phys. Chem. Lett.* **2020**, *11*, 8518–8526. Scaling relationships and volcano plots in homogeneous catalysis.

Anand, M. and Nørskov, J. K. *ACS Catal.* **2020**, *10*, 336–345. Scaling relations in homogeneous catalysis: Analyzing the Buchwald–Hartwig amination reaction.

Bhaskararao, B.; Singh, S.; **Anand, M**. ; Verma, P.; Prakash, P.; Athira, C.; Malakar, S.; Schaefer III, H. F. and Sunoj, R. B. *Chem. Sci.* **2020**, *11*, 208–216. Is silver a mere terminal oxidant in palladium catalyzed C–H bond activation reactions?

Anand, M.; Siahrostami, S. and Nørskov, J. K. *ChemCatChem* **2018**, *10*, 5505–5510. Exploring the effect of gold support on the oxygen reduction reaction activity of metal porphycenes.

Anand, M.; Sunoj, R. B. and Schaefer III, H. F. *ACS Catal.* **2016**, *6*, 696–708. Palladium–Silver cooperativity in an aryl amination reaction through C–H functionalization.

Anand, M.; Fernandez, I.; Schaefer III, H. F. and Wu, J. I. *J. Comp. Chem.* **2015**, 37, 59–63. Hydrogen bond–aromaticity cooperativity in self-assembling 4-Pyridone chains.

Anand, M.; Sunoj, R. B. and Schaefer III, H. F. *J. Am. Chem. Soc.* **2014**, *136*, 5535–5538. Non-innocent additives in a palladium(II)-catalyzed C–H bond activation reaction: Insights into multimetallic active catalysts.

Sunoj, R. B. and **Anand, M**. *Phys. Chem. Chem. Phys.* **2012**, *14*, 12715–12736. Microsolvated transition state models for improved insight into chemical properties and reaction mechanisms.

Anand, M. and Sunoj, R. B. *Organometallics* **2012**, *31*, 6466–6481. Role of explicit solvents in palladium(II)-catalyzed alkoxylation of arenes: An interesting paradigm for preferred outer-sphere reductive elimination over inner-sphere pathway.

Anand, M. and Sunoj, R. B. *Org. Lett.* **2012**, *14*, 4584-4487. Mechanism of cooperative catalysis in a Lewis acid promoted nickel-catalyzed dual C–H activation reaction.

Anand, M. and Sunoj, R. B. *Org. Lett.* **2011**, *13*, 4802-4805. Palladium(II)-catalyzed direct alkoxylation of arenes: Evidence for solvent-assisted concerted metalation deprotonation.

Honors and Awards

Outstanding Graduate Student Award 2015-2016, Northeast Georgia Section American Chemical Society

Dissertation selected to represent University of Georgia in the Council of Graduate Schools (CGS)/Proquest Distinguished Dissertation Award Competition in the field of Physical Sciences, 2016

Undergraduate Research Award (URA) 01 and 03 for two academic years (2010-2012), IIT Bombay.

Awards for academic excellence at **IIT Bombay**:

- Innovation in Science Pursuit for Inspired Research (**INSPIRE**) Merit Scholarship by the Department of Science and Technology, New Delhi, India 2007-2012
- Advinus Merit Scholarship by Chemistry department 2011
- Burjor Goderej Scholarship 2010
- Late Dr. Vasudeo Vithal Bhat Book Grant Award by Chemistry department 2010

Prof. Gowardhan Mehta best poster award in the national meeting of Chemical Research Society of India (CRSI), 2011.

Academic Proficiency Award in Computer Science by the Central Board of Secondary Education (CBSE) in 2005-06

Sahara India Scholarship for excellent academic performance by the Government of Jharkhand state in India, 2004

Conferences and Presentations

Poster selected for Lightning Poster session at the **Reaction mechanisms in catalysis: Faraday Discussion** in February, 2021

Oral presentation at **2020 AIChE Annual Meeting** in November, 2020

Toyota Research Institute Accelerated Materials Design and Discovery (AMDD) Conference in Boston (2017, 2019), Bay Area (2018), and virtual in (2020)

Oral presentation at the **International Conference on Theoretical Aspects of Catalysis** in UCLA campus, Los Angeles, California, USA in 2018

10th Congress of the World Association of Theoretical and Computational Chemists (WATOC) held at Santiago in Chile

Southeastern Theoretical Chemistry Association (SETCA) held at Emory University, Atlanta GA in 2014

National meeting of the Chemical Research Society of India (CRSI, equivalent to the ACS National Meetings in US) held at Bhubaneswar, India in 2011

Training and Workshops

Atomic Simulation Environment (ASE) Workshop at the Chalmers University of Technology in Gothenburg, Sweden, 2019

SurfCat Summer School on the **Science of Sustainable Fuels and Chemicals** at the Kysthusene Gilleleje, in Denmark and the CAMD Summer School on Electronic Structure Theory and Materials Design in Hillerød in 2018.

SUNCAT Summer Institute 2017 on **Fundamentals and Applications of Heterogeneous Catalysis** at the Stanford University

Independent Reviewer

Journal of Computational Chemistry (since 2020)
Nature Communications Chemistry (since 2020)
WIRES Computational Molecular Science (since 2019)
ACS Omega (since 2018)
Physical Chemistry Chemical Physics (since 2015)
RSC Advances (since 2015)

Teaching Experiences

Teaching Assistant for following courses:

- Lecturer and TA for Masters level course – Concepts in heterogeneous catalysis and applications to energy conversion (10339) at the DTU, Autumn 2020
- Freshmen chemistry lab course (CHEM 1212L) at the UGA, Spring 2013
- Freshmen chemistry course CH103 (Chemistry-I) at the IIT Bombay from Fall, 2011
- Computational Chemistry workshop at MG University in Kottayam, Kerala, 2012

Lecturer for summer interns and graduate students at CCQC, UGA on basis sets and Density Functional Theory in 2015

Additional Academic Experiences

Project coordinator for Toyota Research Institute-DTU collaboration since August 2018

Trainees for past and current projects:

- Christina S. Abraham (post-doc in Nørskov group)
- Manajit Das (PhD student in Sunoj group)
- Santanu Malakar (PhD candidate, Rutgers University)

References

Prof. Jens K. Nørskov
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Technical University of Denmark (and Stanford University)
2800 Lyngby, Denmark
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Prof. Henry F. Schaefer III
PhD Advisor
Center for Computational and Quantum Chemistry
University of Georgia Athens
Athens, GA 30602, USA
E-mail: ccq@uga.edu

Prof. Raghavan B. Sunoj
Undergraduate Advisor
IIT Bombay
Mumbai, 400076, India
E-mail: sunoj@chem.iitb.ac.in