Megha Anand

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EDUCATION

PhD in Chemistry August 2012 – May 2016
University of Georgia Athens, GA USA
Center for Computational Quantum Chemistry
Thesis: Theoretical studies on the role of silver salt additives in palladium catalysis
Advisor: Prof. Henry F. Schaefer III
Thesis Committee: (late) Prof. Paul von Ragué Schleyer, Prof. Eric Ferreira, Prof. Shanta Dhar

5-year Integrated M.Sc. in Chemistry (Major) August 2007 – April 2012
Indian Institute of Technology Bombay, Mumbai, India
Master's thesis: DFT studies on mechanism of transition metal catalysed double C–H activation reactions
Advisor: Prof. Raghavan B. Sunoj
Minor: Biosciences and Bioengineering

RESEARCH INTERESTS

Computational Chemistry, Heterogeneous and Homogeneous Catalysis, Materials Discovery, Reaction Mechanisms, Method Development in Catalysis, Machine Learning

PROFESSIONAL APPOINTMENTS

- **Postdoctoral Associate** August 2018 - Present
  Technical University of Denmark
  Catalysis Theory Center
  Advisor: Prof. Jens K. Nørskov
  Projects: *In silico* catalyst discovery for electrochemical N_2 oxidation and O_3 formation
  Development of new methods for homogeneous catalysis using data intensive approaches
  Computational study on doped oxides as stable materials for oxygen reduction reaction

- **Postdoctoral Associate** January 2017 - July 2018
  Stanford University
  SUNCAT Center for Surface Science and Catalysis
  Advisor: Prof. Jens K. Nørskov
  Project: Computational study of oxygen reduction reaction on gold-supported metal porphycenes

- **Education Program Specialist** May 2016 - July 2016
  University of Georgia Athens, GA
  Center for Computational Quantum Chemistry
  Project: Assisted in organizing CCQC summer school

- **Junior Research Fellow** May 2012 - July 2012
  Indian Institute of Technology Bombay, Mumbai, India
  Computational Chemistry Group
  Advisor: Prof. Raghavan B. Sunoj
  Project: Mechanism of Ni-catalyzed dual C–H activation reactions

16. Li, H.; Abraham, C. S.; **Anand, M.**; Cao, A.; Nørskov, J. K. *J. Phys. Chem. Lett.* **2022**, *13*, 2057–2063. Opportunities and challenges in electrolytic propylene epoxidation. [1]
15. **Anand, M.**; Abraham, C. S. and Nørskov, J. K. *Chem. Sci.* **2021**, *21*, 6442–6448. Electrochemical oxidation of molecular nitrogen to nitric acid – towards a molecular level understanding of the challenges. [11]
14. Li, H.; Kelly, S.; Guevarra, D.; Wang, Z.; Wang, Y.; Haber, J. A.; **Anand, M.**; Gunasooriya, G. T. K. K.; Abraham, C. S.; Vijay, S.; and Nørskov, J. K. *Nat. Catal.* **2021**, *4*, 463–468 Analysis of limitations in the oxygen reduction activity of transition metal oxide surfaces. [38]
13. **Anand, M.**; Baletto, F.; Bugaev, A.; Catlow, R.; Claeys, M.; Conway, M.; Davidson, M.; Davies, P. *et al. Faraday Discuss.* **2021**, *229*, 131. Theory: general discussion.
12. **Anand, M.**; Beale, A. M.; Boronat, M.; Bowker, M.; Bugaev, A. L.; Bukhtiyarov, V. I. *et al. Faraday Discuss.* **2021**, *229*, 378. Advanced approaches: general discussion.
11. **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. [11]
10. **Anand, M.** and Nørskov, J. K. *ACS Catal.* **2020**, *10*, 336–345. Scaling relations in homogeneous catalysis: Analyzing the Buchwald–Hartwig amination reaction. [23]
9. 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? [34]
8. **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. [4]
7. **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. [60]
6. **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. [15]
5. **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. [116]
4. 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. [85]
3. **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. [40]
2. **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. [28]
1. **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. [60]

MANUSCRIPTS IN PREPARATION/UNDER REVIEW

1. Abraham, C. S.†; **Anand, M.**† and Nørskov, J. K. **2021**. Analysing oxygen reduction electrocatalysis on Niobium oxide (110) by transition-metal doping. (*under review*)
2. Burke-Stevens, M.; **Anand, M.**; Kreider, M.; Price, E. K.; Zeledon, J. Z.; Peng, J.; Li, H.; Gregoire, J. M.; Hummelshøj, J.; Jaramillo, T. F.; Nørskov, J. K.; Yuriy Roman, Y.; Shao-Horn, Y.; Storey, B.; Suram, S.; Torrisi, S. B.; Montoya, J.; **2022**. New challenges in oxygen reduction catalysis: a consortium retrospective to inform future research. (*under review*)
3. **Anand, M.** and Nørskov, J. K. **2021**. Doping stable binary oxides for improved ORR activity.
4. **Anand, M.** and Nørskov, J. K. **2021** Understanding the role of perchlorates in electrochemical O_3 formation on $PtO_2(110)$.

HONORS AND AWARDS

- **Outstanding Oral contribution (third position) 2022** 2022
  CEHC-2 Cutting-Edge Homogeneous Catalysis meeting, Leipzig Germany

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

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

- **Undergraduate Research Award (URA 01)** 2010 – 2011
  Indian Institute of Technology Bombay

- **Undergraduate Research Award (URA 03)** 2011 – 2012
  Indian Institute of Technology Bombay

- **Innovation in Science Pursuit for Inspired Research Merit Scholarship** 2007 – 2012
  Department of Science and Technology, New Delhi, India

- **Advinus Merit Scholarship** 2011
  Chemistry Department, Indian Institute of Technology Bombay

- **Burjor Goderej Scholarship** 2010
  Chemistry Department, Indian Institute of Technology Bombay

- **Late Dr. Vasudeo Vithal Bhat Book Grant Award** 2010
  Chemistry Department, Indian Institute of Technology Bombay

- **Prof. Gowardhan Mehta best poster award** 2011
  National meeting of Chemical Research Society of India (CRSI)

- **Academic Proficiency Award in Computer Science** 2005 – 2006
  Central Board of Secondary Education (CBSE)

- **Sahara India Scholarship for academic excellence** 2004
  Government of Jharkhand state in India

CONFERENCES AND PRESENTATIONS

9. Invited communication at the **WATOC 2020**, the 12th Triennial Congress of the World Association of Theoretical and Computational Chemists to be held from July 3 to 8, 2022 in Vancouver

8. Keynote lecture at the **240th Electrochemical Society Meeting** held virtual on October 10-14, 2021

7. Poster selected for Lightning Poster session at the **Reaction mechanisms in catalysis: Faraday Discussions** held in February, 2021

6. Oral presentation at the **2020 AIChE Annual Meeting** in November, 2020

5. Poster presentation at **Toyota Research Institute Accelerated Materials Design and Discovery (AMDD) Conference** in Boston (2017, 2019), Bay Area (2018), and virtual in (2020)

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

3. Poster presentation at the **10th Congress of the World Association of Theoretical and Computational Chemists (WATOC)** held at Santiago in Chile in 2014

2. Poster presentation at the **Southeastern Theoretical Chemistry Association (SETCA)** held at the Emory University, Atlanta GA in 2014

1. Poster presentation at the **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** 2019
  Chalmers University of Technology in Gothenburg, Sweden
- **SurfCat Summer School on Science of Sustainable Fuels and Chemicals** 2018
  Organized by the Technical University of Denmark in Gilleleje, Denmark
- **CAMD Summer School on Electronic Structure Theory and Materials Design** 2018
  Organized by the Technical University of Denmark in Hillerød, Denmark
- **Summer Institute on Fundamentals and Applications of Heterogeneous Catalysis** 2017
  Organized by the SUNCAT Center for Surface Science and Catalysis at the Stanford University in Palo Alto, CA USA

TEACHING AND MENTORING EXPERIENCES

- **Technical University of Denmark** (Lecturer and Teaching Assistant)
  – Concepts in heterogeneous catalysis and applications to energy conversion (10339) Fall 2021
  – Concepts in heterogeneous catalysis and applications to energy conversion (10339) Autumn 2020
- **University of Georgia Athens, GA USA** (TA)
  – Freshmen chemistry lab course (CHEM 1212L) Spring 2013
  – Lecturer for summer interns on basis sets and Density Functional Theory Summer 2015
- **Indian Institute of Technology Bombay** (TA)
  – Freshmen chemistry course CH103 (Chemistry-I) Fall 2011
  – Hands-on Computational Chemistry workshop at Mahatma Gandhi University in Kottayam, Kerala India 2012
- **Trainees** for past and current projects
  1. Christina S. Abraham (post-doc in Prof. Nørskov group)
  2. Manajit Das (PhD student in Prof. Sunoj group)
  2. Santanu Malakar (undergraduate student in Prof. Sunoj group) currently a PhD candidate at the Rutgers University

PROFESSIONAL SERVICE

- **Peer 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)
- **Invited guest at the Organic Letters Editorial Advisory Board Meeting** at Palace Hotel in San Francisco on April 2, 2017.
- **Project coordinator** for Toyota Research Institute – DTU collaboration since August 2018

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