



Vishal Agarwal

Assistant Professor



FB 466, Faculty Building
IIT Kanpur, Kanpur 208016,
Uttar Pradesh, India.



+91 (512) 259-6895



<https://www.iitk.ac.in/che/faculty/va.htm>



vagarwal@iitk.ac.in

Biographical Sketch

Vishal Agarwal is presently working as an assistant professor in the department of chemical engineering at Indian Institute of Technology Kanpur, India. Previously, he worked as a postdoctoral scholar with Prof. Horia Metiu at University of California, Santa Barbara. He obtained his PhD in Chemical Engineering from University of Massachusetts, Amherst. He has a Master's degree in Chemical Engineering from IIT Bombay and a undergraduate degree in Chemical Engineering from Panjab University, Chandigarh. From 2003 to 2004, he worked as process design engineer in Technip KT India Ltd. His research on cellulose pyrolysis was highlighted in North American Clean Energy and BioDigest. He has also been awarded Best Master's Research Thesis Award for his research efforts on reactive distillation.

Interests

Catalysis, Biofuels, Nucleation, Gas-Surface and Liquid-Surface Interactions, Molecular Simulation, Ab initio Molecular Dynamics, Density Functional Theory, Rare-Event Simulations, Reaction Rate Theory, Statistical Mechanics.

Education

- Ph.D. Chemical Engineering** Sept'06 – May'12
University of Massachusetts, Amherst, USA (UMass)
Doctoral Thesis: *Modeling Material Transformations in Biorefinement*
- M.S. Chemical Engineering (Student Excellence Award)** Aug'04 – July'06
Indian Institute of Technology, Bombay (IITB)
Master's Thesis: *Attainable Regions of Reactive Distillation*
- B.S. Chemical Engineering (Honors)** July'99 – May'03
Panjab University, Chandigarh, India (PU)
Bachelor's Thesis: *Design of Ethylene Oxide Production Unit*

Appointments

- Assistant Professor of Chemical Engineering** Jan'17 – current
Indian Institute of Technology, Kanpur, India (IITK)
- PostDoctoral Scholar** Jun'12 – Dec'16
University of California, Santa Barbara, USA (UCSB)
Advisor: *Prof. Horia Metiu*
- Process Design Engineer** Sept'03 – May'04
Technip KT India Ltd.
- Summer Intern** May'02 – July'02
Indian Oil Corporation Ltd. (IOCL), Baroda, India

Awards and Honors

- Research on molten metals highlighted in **ScienceDaily**, **AmarUjala**, **GreenCarCongress**, **ResearchMatters** and **ChemistryWorld**.
- **Ramanujan Fellowship**, 2017.
- Research on cellulose decomposition highlighted in **BioBased Digest** and **North American Clean Energy**.
- RG Madhudhane M. Tech. **Best Masters Research Thesis Award**, IITB, 2006.
- **1st Prize** in Technical Paper Presentation, Eureka-2002, PU, 2002.

Journal Publications [hindex = 12; i10-index = 14]

17. Horia Metiu, **Vishal Agarwal**, Henrik H. Kristoffersen, *The Role of Computations in Catalysis*, Reviews in Computational Chemistry 31, 2018, 171-196.
16. David C. Upham, **Vishal Agarwal**, Alexander Khechfe, Zachary R. Snodgrass, Michael J. Gordon, Horia Metiu, and Eric W. McFarland, *Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon*, Science 358 (6365), 2017, 917-921.
15. **Vishal Agarwal** and Horia Metiu, *Oxygen Vacancy Formation on α -MoO₃ Slabs and Ribbons*, The Journal of Physical Chemistry C 120 (34), 2016, 19252-19264.
14. **Vishal Agarwal** and Horia Metiu, *Energy of Oxygen-Vacancy Formation on Oxide Surfaces: Role of the Spatial Distribution*, The Journal of Physical Chemistry C 120 (4), 2016, 2320-2323.
13. **Vishal Agarwal** and Horia Metiu, *Hydrogen Abstraction Energies and Ammonia Binding to BEA, ZSM-5, and α -Quartz Doped with Al, Sc, B, or Ga*, The Journal of Physical Chemistry C 119 (28), 2015, 16106-16114.
12. **Vishal Agarwal** and Baron Peters, *Nucleation near the eutectic point in a Potts-lattice gas model*, The Journal of chemical physics 140 (8), 2014, 084111.



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11. **Vishal Agarwal** and Baron Peters, *Solute precipitate nucleation: A review of theory and simulation advances*, *Advances in Chemical Physics* 155, 2014, 97-160.
10. **Vishal Agarwal**, Paul J. Dauenhauer, George W. Huber, and Scott M. Auerbach, *Ab initio dynamics of cellulose pyrolysis: Nascent decomposition pathways at 327 and 600 C*, *Journal of the American Chemical Society* 134 (36), 2012, 14958-14972.
9. **Vishal Agarwal**, George W. Huber, W. Curtis Conner Jr, and Scott M. Auerbach, *Simulating infrared spectra and hydrogen bonding in cellulose I β at elevated temperatures*, *The Journal of chemical physics* 135 (13), 2011, 134506.
8. **Vishal Agarwal**, W. Curtis Conner Jr, and Scott M. Auerbach, *DFT Study of Nitrogen-Substituted FAU: Effects of Ion Exchange and Aluminum Content on Base Strength*, *The Journal of Physical Chemistry C* 115 (1), 2010, 188-194.
7. **Vishal Agarwal**, George W. Huber, W. Curtis Conner, and Scott M. Auerbach, *Kinetic stability of nitrogen-substituted sites in HY and silicalite from first principles*, *Journal of Catalysis* 270 (2), 2010, 249-255.
6. **Vishal Agarwal**, George W. Huber, W. Curtis Conner, and Scott M. Auerbach, *DFT study of nitrated zeolites: Mechanism of nitrogen substitution in HY and silicalite*, *Journal of Catalysis* 269 (1), 2010, 53-63.
5. Karl D. Hammond, Fulya Dogan, Geoffrey A. Tompsett, **Vishal Agarwal**, W. Curtis Conner Jr, Clare P. Grey, and Scott M. Auerbach, *Spectroscopic signatures of nitrogen-substituted zeolites*, *Journal of the American Chemical Society* 130 (45), 2008, 14912-14913.
4. **Vishal Agarwal**, Suman Thotla, Rupinder Kaur, and Sanjay M. Mahajani, *Attainable regions of reactive distillation. Part II: Single reactant azeotropic systems*, *Chemical Engineering Science* 63 (11), 2008, 2928-2945.
3. **Vishal Agarwal**, Suman Thotla, and Sanjay M. Mahajani, *Attainable regions of reactive distillation. Part I: Single reactant non-azeotropic systems*, *Chemical Engineering Science* 63 (11), 2008, 2946-2965.
2. Suman Thotla, **Vishal Agarwal**, and Sanjay M. Mahajani, *Aldol condensation of acetone with reactive distillation using water as a selectivity enhancer*, *Industrial & Engineering Chemistry Research* 46 (25), 2007, 8371-8379.
1. Suman Thotla, **Vishal Agarwal**, and Sanjay M. Mahajani, *Simultaneous production of diacetone alcohol and mesityl oxide from acetone using reactive distillation*, *Chemical Engineering Science* 62 (18), 2007, 5567-5574.

Journal Papers In-Preparation/Submitted

2. **Vishal Agarwal** and Horia Metiu, *Exact Classical Adsorption and Desorption Rates of a Diatomic Molecule*, 2017, Submitted.
1. **Vishal Agarwal** and Horia Metiu, *CH₄ Dissociation in Molten Pt-Sn and Ni-Bi*, 2017, in-preparation.

Conference Proceedings

1. Vishal Agarwal, Suman Thotla and Sanjay M. Mahajani, *Selectivity Engineering with Reactive Distillation: Determination of Attainable Region*, in *Distillation & Absorption* 2006, 73-87.

Invited Talks

9. **Vishal Agarwal***, *Modeling Material Transformations at High Temperatures*, invited by HBTI, Kanpur, Uttar Pradesh, India, July 2018.
8. **Vishal Agarwal***, *Molecular Modeling of Cellulose Pyrolysis*, invited by Indian Institute of Technology (IIT) Delhi, India, Mar. 2016.
7. **Vishal Agarwal***, *Molecular Modeling of Cellulose Pyrolysis*, invited by National Chemical Laboratories (NCL) Pune, India, Mar. 2016.
6. **Vishal Agarwal***, *Molecular Modeling of Cellulose Pyrolysis*, invited by Indian Institute of Technology (IIT) Bombay, India, Mar. 2016.



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5. **Vishal Agarwal***, *Molecular Modeling of Cellulose Pyrolysis*, invited by Indian Institute of Technology (IIT) Kanpur, India, Mar. 2016.
4. **Vishal Agarwal***, *Molecular Modeling of Cellulose Pyrolysis*, invited by Honeywell UOP, Chicago, USA, Oct. 2015.
3. **Vishal Agarwal***, *Modeling of Nitrogen-Substituted Zeolites: Synthesis, Stability and Base Characteristics*, invited by Honeywell UOP, Chicago, USA, Aug. 2015.
2. **Vishal Agarwal***, *Modeling Material Transformation in Bio-refinement*, invited by Prof. Baron Peters, UCSB, Dec. 2011.
1. **Vishal Agarwal***, *Modeling Material Transformation in Bio-refinement*, invited by Prof. William H. Green, MIT, Nov. 2011.

Conference Presentations

14. **Vishal Agarwal***, Paul J. Dauenhauer, G. W. Huber, and Scott M. Auerbach, *Nascent Decomposition Pathways of Cellulose from First Principles*, AIChE annual meeting, Pittsburg, USA, October 2012.
13. **Vishal Agarwal***, W. Curtis Conner, G. W. Huber, and Scott M. Auerbach, *Modeling of Cellulose Pyrolysis using Molecular Dynamics*, AIChE annual meeting, Utah, USA, November 2010.
12. **Vishal Agarwal***, W. Curtis Conner, G. W. Huber, and Scott M. Auerbach, *Optimizing Base Strength of Nitrogen-Substituted FAU Zeolite*, AIChE annual meeting, Utah, USA, November 2010.
11. **Vishal Agarwal***, W. Curtis Conner, G. W. Huber, and Scott M. Auerbach, *Kinetic Stability of Nitrogen-Substituted Zeolites from First Principles*, AIChE annual meeting, Utah, USA, November 2010.
10. George W. Huber*, Joungmo Cho, Torren Carlson, Robert Coolman, **Vishal Agarwal**, Saba Almalkie, Yenhan Lin, Scott Auerbach, Stephen de Bruyn Kops, TJ Mountziaris, William C Conner, Jeffrey M Davis and Paul Dauenhauer, *Green aromatics by catalytic fast pyrolysis of lignocellulosic biomass*, ACS, Washington, USA, Oct. 2010.
9. **Vishal Agarwal***, W. Curtis Conner, G. W. Huber, and Scott M. Auerbach, *Modeling of Synthesis, Stability and Base Characteristics of Nitrogen Substituted HY and Silicalite*, AIChE annual meeting, Tennessee, USA, November 2009.
8. Scott M. Auerbach* and **Vishal Agarwal**, *Parallel Chain-of-States Method for Finding Saddle Point in Materials Chemistry: Designing Bio-Fuel Catalysts*, BECAT-IBM Workshop on High Performance Computational Science and Engineering, UConn, USA, December 2008.
7. **Vishal Agarwal***, George W. Huber, W. Curtis Conner Jr. and Scott M. Auerbach, *Mechanistic Modeling of Nitrogen Incorporation Inside Zeolites*, NECZA, UPenn, USA, December 2008.
6. Karl D. Hammond*, Fulya Dogan, Geoffrey A. Tompsett, Murad Gharibeh, **Vishal Agarwal**, W. Curtis Conner, Clare P. Grey, and Scott M. Auerbach, *The Spectroscopic Signature Nitrogen-Substituted Zeolites*, AIChE annual meeting, Philadelphia, USA, November 2008.
5. **Vishal Agarwal**, Suman Thotla, Rupinder Kaur, M. Chalakova, H. Freund, Kai Sundmacher and Sanjay M. Mahajani*, *Attainable Regions of Reactive Distillation*, Indo-German Workshop on Advances in Reaction and Separation Processes, Madras, India, 18-20 February 2008.
4. Suman Thotla*, **Vishal Agarwal** and Sanjay M. Mahajani, *Aldol Condensation of Acetone with Reactive Distillation using Water as Selectivity Enhancer*, CAMURE-6 & ISMR-5, NCL-Pune, January 2007.
3. Rupinder Kaur*, **Vishal Agarwal**, Suman Thotla and Sanjay M. Mahajani, *Attainable Regions of Reactive Distillation: Multiple azeotrope systems and systems with inerts*, CHEMCON 2006, Ankleshwar, India, December 2006.



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2. **Vishal Agarwal**, Suman Thotla and Sanjay M. Mahajani*, *Selectivity Engineering with Reactive Distillation: Determination of Attainable Region*, Distillation & Absorption, UK, September 2006.

1. Suman Thotla*, **Vishal Agarwal** and Sanjay M. Mahajani, *Simultaneous Production of Diacetone Alcohol and Mesityl Oxide from Acetone using Reactive distillation*, ISCRE-19, Potsdam/Berlin, Germany, September 2006.

Professional Service

Professional Organizations

North England Catalysis Society (NECS), American Institute of Chemical Engineers (AIChE), American Chemical Society (ACS).

Conference Chair

Recent Advances in Modeling Rare Events (Dec'17); 9th International Symposium on Group Five Elements (Nov'17).

Journal Reviewer

Nature Communications, Journal of Physical Chemistry, Langmuir, International Journal of Molecular Science, Environmental Science and Technology, Journal of Chemical Sciences, Applied Physics Letters, Materials Science in Semiconductor Processing, Canadian Journal of Chemistry.

Teaching and Mentoring

Phd Thesis Supervised/Supervising

1. "Development of Catalyst for CO₂ Utilization: Experiments and Modeling"— Undertaken by Ragamaye Tigiripalli (co-supervised with Prof. Goutam Deo).
2. "Predictive Modeling of Hydrodeoxygenation Catalyst for Biofuel Upgrading"— Undertaken by Abir Lal Bose.
3. "Computational and Experimental Studies of Enzymatic Catalysis"— Undertaken by Neeraj Kumar Kanaujia (co-supervised with Prof. Raghvendra Singh).

Master's Thesis Supervised/Supervising

1. "Simulating potential drop and capacitance of an electrical double layer"— Undertaken by Shilpa Kumari (2018–2019).
2. "Probing Role of Ions in Aqueous Phase ATP Hydrolysis"— Undertaken by Raghav Saxena (2018–2019); co-supervised with Prof. Raghvendra Singh.
3. "Probing Role of Water in ATP Hydrolysis in Aqueous Phase"— Undertaken by Sai Phani Kumar (2018–2019); co-supervised with Prof. Raghvendra Singh.
4. "Developing non-polarizable Force-Field for Water and Aqueous NaCl Solution"— Undertaken by Jaishri Jain (2017–2018).

Undergraduate Project Supervised/Supervising

1. "Evaluating water force-fields in liquid phase using experimental radial distribution function"— Undertaken by Pranshu Tripathi (Fall 2018).
2. "Modeling CH₄ decomposition in Molten Tellurium"— Undertaken by Shivali Agrawal (Fall 2018).
3. "Evaluating water force-fields in gas-phase using accurate quantum chemical calculations"— Undertaken by Ashar Ahmad (Fall 2017).



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Undergraduate Research Mentored/Mentoring

Pranshu Tripathi (Dec'17-current); Shivali Agrawal (Feb'18-current); Parth Chhapparwal (May'18-July'18); Deeksha Yadav (Mar'18-July'18); Harshit Verma (April'18-July'18); Amartya Kumar Prusty (Oct'17-July'18); Sarthak Gupta (Dec'17-July'18); Akhil Dubey (May'18-July'18); Debjyoti Bhakta (May'18-July'18); Ashar Ahmad (May'17-Dec'17); Dharmendra (May'17-July'17); Nikhil Chole (May'17-July'17); Shivam (May'17-July'17); Deepak Yadav (May'17-July'17); Jaswinder Singh (May'17-July'17); Sandhya Raj (May'17-July'17); Yingying Lin (Oct'16-Jun'17); Chris Yuan (Jan'13-Jan'14); Tyler Jordison (May'09-Aug'09); Rachel Shirron (May'08-Aug'08).

Course Instructor

Practical Introduction to Quantum Chemical Methods (Spring 2018); Chemical Process Simulation Lab (Fall 2017, Fall 2018).

Guest Lecturer

Heterogeneous Catalysis (Prof. Goutam Deo); Statistical Mechanics (Prof. Scott M. Auerbach); Chemical Process Design (Prof. George W. Huber).

Tutor

Computational Methods in Engineering (Aug'17-Nov'17); Atoms, Photons and Molecules (Jan'17-May'17).

Teaching Assistant

Thermodynamics; Chemical Process Design; Chemical Reaction Engineering; Conceptual Design of Selected Separation Processes; Advanced Transport Phenomena; Safety in Chemical Industry; Mass Transfer.