Vishal Agarwal

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Biographical Sketch

Vishal Agarwal is presently working as an associate professor in the department of chemical engineering at Indian Institute of Technology Kanpur, India. Previously, he worked as a postdoctoral scholar 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 Universtiy, 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 intio 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.E. Chemical Engineering (Honors) — July'99 – May'03
Panjab University, Chandigarh, India (PU)
Bachelor's Thesis: *Design of Ethylene Oxide Production Unit*

Appointments

Associate Professor of Chemical Engineering — July'22 – current
Indian Institute of Technology, Kanpur, India (IITK)

Adjunct Professor of Sustainable Energy and Engineering — Jan'21 – current
Indian Institute of Technology, Kanpur, India (IITK)

Assistant Professor of Chemical Engineering — Jan'17 – Jun'22
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

- Senate Chairman's Commendation for Teaching "Chemical Reaction Engineering", 2022.
- Senate Chairman's Commendation for Teaching "Chemical Engineering Thermodynamics", 2022.
- Senate Chairman's Commendation for Teaching "Chemical Engineering Thermodynamics", 2021.
- 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.

Publications [hindex = 14; i10-index = 15]

31. M. Dinachandra Singh, Deepak Kumar Gorai, Kumar Brajesh, Pragati Singh, Vishal Ranawade, Ajay Vijay Shinde, M. Jareer, Raju Gupta, Ashish Garg, **Vishal Agarwal**, Kanwar S. Nalwa*, *Ruthenium doping of NASICON electrolyte augments the performance of solid-state sodium-ion batteries*,Chemical Engineering Journal 489, 2024, 151330.

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30. Nikil Surya R, Sunny Kumar Bhagat, Horia Metiu*, **Vishal Agarwal***, *Activation of Methane in Vapor and Molten Sodium Catalyst*, Journal of Physical Chemistry C 128 (8), 2024, 3233-3241.
29. Abir Lal Bose, Sayali Ramteke, Goutam Deo, **Vishal Agarwal***, *Structures and reactivity of monomeric MoO_x moieties supported on ZrO_2 (111) slab: A DFT study*, Journal of Catalysis 429, 2024, 115267.
28. Sajal Kanti Dutta, Baljit Singh, Horia Metiu*, **Vishal Agarwal***, *Increase of the Catalytic Activity of Molten Salts by Doping: Methane Activation*, Journal of Physical Chemistry C 128 (1), 2024, 123-128.
27. Aditya Goyal, **Vishal Agarwal***, *Rate-Enhancing Role of Water in H-BEA and Sn-BEA for Keto-Enol Tautomerization of Acetone: A DFT Study*, Journal of Physical Chemistry C 127 (46), 2023, 22618-22628.
26. Ragamaye Tigiripalli, **Vishal Agarwal***, Goutam Deo*, *Case Studies on the Advances in the Raman Characterization of Heterogeneous Catalysts*, Springer Handbook of Advanced Catalyst Characterization, 2023, 111-129.
25. Krishna Jaiswal, Horia Metiu*, **Vishal Agarwal***, *The Desorption Rate at Liquid-Solid Interface*, arxiv 2211.08122, 2022.
24. Abir Lal Bose and **Vishal Agarwal***, *Oxygen Healing and CO_2/H_2/Anisole Dissociation on Reduced Molybdenum Oxide Surfaces Studied by Density Functional Theory*, ChemPhysChem 23, 2022, e202200510.
23. Sajal K. Dutta, Smita Ghosh, Horia Metiu* and **Vishal Agarwal***, *Nascent Decomposition Pathways of CH_4 in Gas Phase Metal Hallides*, Journal of Physical Chemistry A 126 (35), 2022, 5900-5910.
22. Sajal K. Dutta, and **Vishal Agarwal***, *DFT Study of Phenol Alkylation with Propylene in H-BEA in the Absence and Presence of Water*, Reaction Chemistry & Engineering 6(12), 2021, 2315-2326. **Published in "Emerging Investigator Series"**.
21. Raghav Saxena, A. V. B. K. Sai Phani Kumar, Raghvendra Singh*, and **Vishal Agarwal***, *Ab initio Dynamics of Gas-phase and Aqueous-phase Hydrolysis of ATP*, 2021, International Journal of Quantum Chemistry 121(10), 2021, e26615.
20. **Vishal Agarwal***, and Horia Meitu*, *Rates of adsorption and desorption: Entropic contributions and errors due to mean-field approximations*, The Journal of chemical physics 150 (18), 2019, 184702.
19. Horia Metiu*, **Vishal Agarwal**, Henrik H. Kristoffersen, *Oxide Catalysis*, Handbook of Materials Modeling, 2018, 1-12.
18. Horia Metiu*, **Vishal Agarwal**, Henrik H. Kristoffersen, *The Role of Computations in Catalysis*, Reviews in Computational Chemistry 31, 2018, 171-196.
17. 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.
16. **Vishal Agarwal** and Horia Metiu*, *Oxygen Vacancy Formation on α-MoO_3 Slabs and Ribbons*, The Journal of Physical Chemistry C 120 (34), 2016, 19252-19264.
15. **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.
14. **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.
13. **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.
12. **Vishal Agarwal** and Baron Peters*, *Solute precipitate nucleation: A review of theory and simulation advances*, Advances in Chemical Physics 155, 2014, 97-160.

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Interests

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

11. **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.
10. **Vishal Agarwal**, George W. Huber, W. Curtis Conner Jr, and Scott M. Auerbach*, *Simulating infrared spectra and hydrogen bonding in cellulose $I\beta$ at elevated temperatures*, The Journal of chemical physics 135 (13), 2011, 134506.
9. **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.
8. **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.
7. **Vishal Agarwal**, George W. Huber, W. Curtis Conner, and Scott M. Auerbach*, *DFT study of nitrided zeolites: Mechanism of nitrogen substitution in HY and silicalite*, Journal of Catalysis 269 (1), 2010, 53-63.
6. 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.
5. **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.
4. **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.
3. 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.
2. 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.
1. **Vishal Agarwal**, Suman Thotla and Sanjay M. Mahajani*, *Selectivity Engineering with Reactive Distillation: Determination of Attainable Region*, in Distillation & Absorption 2006, 73-87.

Journal Papers In-Preparation/Submitted

3. Nikil Surya R., Raju K. Gupta and **Vishal Agarwal***, *Role of Water and Ta-dopant for Photocatalysis of CO_2 on Anatase TiO_2 Surface: A DFT Study*, 2022, in-preparation.
2. Kanishka Charakhwal and **Vishal Agarwal***, *Investigating the Role of H_2O_2 as Oxidant and H_2O as Co-catalyst for Photocatalytic Conversion of Methane to Methanol over A-TiO_2 (101)*, 2022, in-submitted.
1. Jaishri Jain, Shilpa Kumari, Krishna Jaishwal, and **Vishal Agarwal***, *A Functional Force-Field Model for Water based on Gaussian Charges*, 2022, in-preparation.

Invited Talks

14. **Vishal Agarwal***, *Novel Algorithms for Efficient Exploration of Potential Energy Surfaces*, invited by Indian Institute of Technology (IIT) Kanpur, India, April 2024.
13. **Vishal Agarwal***, *CO_2-free Production of H_2 from Methane Pyrolysis in Molten Catalyst: Insights from Ab initio Simulations*, invited by Indo-German Science and Technology Centre (IGSTC), IIT Bombay, India, Feb.2024.
12. Krishna Jaiswal*, Horia Metiu, **Vishal Agarwal**, *Rates of Desorption on a Solid-Liquid Interface*, invited by Theoretical Chemistry Symposium (TCS), IISER Kolkata, India, December 2021.

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11. **Vishal Agarwal***, *Modeling Material Transformation in Bio-refinement*, invited by PPSU, GUJCOST webinar on Renewable Biofuel and Bioenergy in the global energy transformation, Gujarat , India, Oct. 2020.
10. **Vishal Agarwal***, *Rates of adsorption and desorption: Entropic contributions and errors due to mean-field approximations*, invited by IIT, Delhi, New Delhi, India, March 2019.
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 Chemcial 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.
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

35. Subhadeep Dey*, Abir Lal Bose, **Vishal Agarwal**, and Goutam Deo, *Interactive effect of Mo and W over vanadia supported ZrO_2 for oxidative dehydrogenation of propane*, IIChE-CHEMCON, Kolkata, West Bengal, India, December 2023.
34. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *Adaptively accelerated relaxation engine (AARE) for optimizing minimum energy path*, ChEmference, BITS Pilani Goa, India, September 2023. **(Third Prize)**
33. Nikil Surya R*, Sunny Kumar Bhagat, Horia Metiu, and **Vishal Agarwal**, *Modeling methane pyrolysis in vapor and molten sodium catalyst*, ChEmference, BITS Pilani, K. K. Birla Goa Campus, Goa, India , September 2023.
32. Aditya Goyal*, Horia Metiu, and **Vishal Agarwal**, *Ab initio moleculer dynamics study to investigate the role of Ti doping in molten KCI for methane activation*, ChEmference, BITS Pilani, K. K. Birla Goa Campus, Goa, India , September 2023.
31. Abir Lal Bose*, Sayali Ramteke, Goutam Deo, and **Vishal Agarwal**, *A DFT+U study to model slabs of reduced MoO_x and isolated monomeric MoO_x clusters on ZrO_2 for hydrodeoxygenation reaction*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2023.
30. Abir Lal Bose*, Sayali Ramteke, Raghav Singh Thakur, Goutam Deo, and **Vishal Agarwal**, *Modeling the structure of monomeric MoO_x and VO_x clusters supported on ZrO_2 and their interaction with each other*, CHEMTSF, IIT Roorkee, Uttarakhand, India, September 2022.
29. Aditya Goyal*, and **Vishal Agarwal**, *Elucidating the role of water in keto-enol tautomerization of acetone in BEA zeolite*, CHEMTSF, IIT Roorkee, Uttarakhand, India, September 2022.
28. Baljit Singh*, Sajal Kanti Dutta, Horia Metiu, and **Vishal Agarwal**, *Modeling the catalytic role of Fe in a molten $FeCl_3$-KCl Melt for methane decomposition*,CHEMTSF, IIT Roorkee, Uttarakhand, India, September 2022.

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27. Krishna Jaiswal*, Horia Metiu, **Vishal Agarwal**, *Rates of Desorption on a Solid-Liquid Interface*, CHEMTSF, IIT Roorkee, Uttarakhand, India, September, 2022. (**Best oral presentation**)
26. Nikil Surya R*, Raju Kumar Gupta, **Vishal Agarwal** , *Role of water and Ta-dopant on photocatalysis of CO_2*, CHEMTSF, IIT Roorkee, Uttarakhand, India, September 2022.
25. Nikil Surya R*, Sunny Kumar Bhagat*, **Vishal Agarwal**, *Modeling Methane pyrolysis in molten sodium catalyst*, CHEMTSF, IIT Roorkee, Uttarakhand, India, September 2022.
24. Sajal Kanti Dutta*, Baljit Singh, Horia Metiu, **Vishal Agarwal**, *Modeling the catalytic role of Fe in a molten $FeCl_3$-KCl melt for methane decomposition*, CHEMTSF, IIT Roorkee, Uttarakhand, India, September, 2022.
23. Sandra Liz Simon *, Nitin Kaistha, **Vishal Agarwal**, *Developing novel algorithms for exploring potential energy surfaces and reaction pathways*, CHEMTSF, IIT Roorkee, Uttarakhand, India, September, 2022.
22. Ragamaye Tigiripalli*, **Vishal Agarwal**, and Goutam Deo, *DFT Study of CO_2 Activation on Cu(111): Role of Water and Adatoms*, CHEMCON, Bhubaneswar, India, December 2021.
21. Abir Lal Bose* and **Vishal Agarwal**, *Oxygen Healing Energies of Reduced Molybdenum Oxides: A DFT Study*, CHEMCON, Bhubaneswar, India, December 2021.
20. Nikil Surya R*, Raju Kumar Gupta, and **Vishal Agarwal**, *A DFT Study on Adsorption of CO_2 on Pristine, Defective and Ta-doped Anatase (101) Surface*, CHEMCON, Bhubaneswar, India, December 2021.
19. Krishna Jaiswal*, Horia Metiu and **Vishal Agarwal**, *Rates of Desorption on a Solid-Liquid Interface*, CHEMCON, Bhubaneswar, India, December 2021.
18. Krishna Jaiswal*, Horia Metiu, **Vishal Agarwal**, *Rates of Desorption on a Solid-Liquid Interface*, TCS, IISER Kolkata, Kolkata, West Bengal, India, December, 2021.
17. Aditya Goyal*, **Vishal Agarwal**, *Modelling the Role of Water in Sn-BEA Zeolite for Biofuel Upgrading*, CHEMCON, Bhubaneswar, Odisha, India, December 2021.
16. D Chester Upham*, Clarke Palmer, Jiren Zeng, Shizhao Su, **Vishal Agarwal**, Henrik H. Kristoffersen, Michael Gordon, Eric McFarland, Horia Metiu, *Hydrogen production without CO2: Experiments and computations*, ACS, Boston, Massachusetts, USA, August 2018.
15. Horia Metiu*, Eric McFarland, Michael Gordon, **Vishal Agarwal**, David Upham, Henrik Kristoffersen, *Molecular dynamics and possible catalytic chemistry by molten metals or salts*, ACS, San Francisco, California, USA, April 2017.
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.

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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 Catalyts*, 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.
2. **Vishal Agarwal**, Suman Thotla and Sanjay M. Mahajani*, *Selectivity Engineering with Reactive Distillation: Determination of Attainable Region*, Distillation & Absroption, 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, International Journal of Hydrogen Energy, Proceedings of the National Academy of Sciences, India Section A: Physical Sciences, ChemCatChem, Environmental Sustainability, Journal of Physics and Chemistry of Solids, International Journal of Quantum Chemistry.

Miscellaneous

Evaluator for KPIT Sparkle 2021 (May'19); Evaluator for KPIT Sparkle 2020 (Dec'19); Special Guest at KPIT Innovation Council and KPIT Sparkle (Feb'18), Reviewer for ACS Petroleum Research Fund (July'19), Reviewer for DST and NSM (Jan-Feb'21).

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Biographical Sketch

Vishal Agarwal is presently working as an associate professor in the department of chemical engineering at Indian Institute of Technology Kanpur, India. Previously, he worked as a postdoctoral scholar 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 Universtiy, 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 intio Molecular Dynamics, Density Functional Theory, Rare-Event Simulations, Reaction Rate Theory, Statistical Mechanics.

Teaching and Mentoring

Phd Theses Supervised (0)/Supervising (6)

6. "Developing Novel Algorithms For Exploring Potential Energy Surfaces"— Undertaken by Sandra Liz Simon (co-supervised with Prof. Nitin Kaistha; 2021-current).
5. "Experimental and DFT Study of Solid Electrolyte Interfaces"— Undertaken by Joseph Nishanth J. (co-supervised with Prof. Kanwar Singh Nalwa; 2021-current).
4. "Conversion of Polyethylene to H_2 using Molten-metal/Molten-Salt Catalysts"— Undertaken by Rupesh Singh (co-supervised with Prof. Raju Kumar Gupta; 2020-current).
3. "Modeling the Role of Water in Nanoporus Catalysis"— Undertaken by Aditya Goyal (2019-current).
2. "Modeling TiO_2 as Photocatalyst for the conversion of CO_2 to Fuels"— Undertaken by Nikil Surya (co-supervised with Prof. Raju Kumar Gupta; 2019-current).
1. "Predictive Modeling of Hydrodeoxygenation Catalyst for Biofuel Upgrading"— Undertaken by Abir Lal Bose (2018-current).

Master's Theses/Project Supervised (10)/Supervising (5)

15. "Rate Enhancing Role of Dopants in Molten Halide Catalyst"— Undertaken by Hema Punyamoorty (2024-current).
14. "Designing Novel Algorithms for Parallelization of 2D EWALD Summation"— Undertaken by Prateek Kumar Panday (2023-current); co-supervised with Prof. Swarnendu Biswas.
13. "Promotional Effect of Mo and W over Vanadia Supported ZrO_2 Catalyst for ODH of Propane "— Undertaken by Subhadeep Dey (2022-current); co-supervised with Prof. Goutam Deo.
12. "Why Carbon Dioxide Conversion goes up in In-Ni Molten Alloy in Comparison to Pure In Molten Metal"— Undertaken by Abdul Kaish (2022-current).
11. "Experimental Study on Methane Pyrolysis in Molten Metal Halides"— Undertaken by Vikash Kumar Gupta (2022-current); co-supervised with Prof. Himanshu Sharma.
10. "Modeling the Mechanistic Pathways of Anisole Hydro-Deoxygenation on a Mo_2C Surface"— Undertaken by Rishika (2021-2023).
9. "Modeling CH_4 Decomposition in Molten Metal Halides"— Undertaken by Baljit Singh (2021-2023).
8. "Rates of Adsorption/Desorption on a Liquid/Solid Interface"— Undertaken by Krishna Jaiswal (2019-2022).
7. "Interaction Between Monomeric Transition Metal Oxide Clusters Supported on ZrO_2 & TiO_2"— Undertaken by Raghav Singh (2020-2022).
6. "Modeling of MoO_x on ZrO_2 in Oxidizing and Reducing conditions"— Undertaken by Sayali Ramteke (2020-2021).
5. "Modeling the Role of Water in Sn-Beta for Aldol Condensation of Acetone and Formaldehyde "— Undertaken by Aman Gupta (2019–2020).
4. "Investigating an All-Atom Gaussian-Charge Based Water Model for Gas Phase Clusters "— Undertaken by Shilpa Kumari (2018–2019).
3. "Modeling the Role of Water and Ions in ATP Hydrolysis"— Undertaken by Raghav Saxena (2018–2019); co-supervised with Prof. Raghvendra Singh.
2. "Conformational Analysis of ATP in Gas-Phase, Implicit Water, and Explicit Solvent"— Undertaken by Sai Phani Kumar (2018–2019); co-supervised with Prof. Raghvendra Singh.
1. "Development of All-atom Aqueous NaCl Force-Field for Microscopic Simulations of Electrical Double Layer"— Undertaken by Jaishri Jain (2017–2018).

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PostDoctoral Fellows Supervised (3)/Supervising (2)

5. "Modelling the Chemistry of Solvated Electrons in Metal Doped Metal Halides"— Undertaken by Dr. Deepak Gorai (2023-current).
4. "Modelling CH_4 Decomposition in Molten Mg and Mg-Zn Alloys"— Undertaken by Dr. Juhi Srivastava (2022-current).
3. "Modelling the Structure and Nature of Catalytic Sites on Molybdenum-oxycarbide Supported by TiO_2 in Reduced Conditions"— Undertaken by Dr. Mahesh Dutt Bhatt (2022).
2. "Nascent Decomposition Pathways of CH_4 in Gas-Phase Hallide Catalyst"— Undertaken by Dr. Smita Ghosh (2020-2021).
1. "Modeling the Role of Water in Phenol Alkylation using H-BEA Zeolite" and "Modeling the Role of $FeCl_3$ in Molten-Hallide Catalysis"— Undertaken by Dr. Sajal Kanti Dutta (2019-current).

Undergraduate Project Supervised (10)

10. "Modeling Gas-phase and Molten Na Catalysis for CH_4 Decompostion"— Undertaken by Sunny Kumar Bhagat (Spring 2022).
9. "Modeling Homogeneous Nucleation of CO_2 Clathrates"— Undertaken by Vrahant Nagoria (Fall 2021).
8. "Modeling the Role of monomeric ZrO_2 clusters on Cu Surfaces for CO_2 Hydrogenation"— Undertaken by Ayushi Goyal (Fall 2020).
7. "Modeling the Role of Water in Methane Dissociation on TiO_2 Surfaces"— Undertaken by Kanishka (Summer, Fall 2020).
6. "Modeling MoO_x clusters on TiO_2 Support for Bio-oil Upgrading"— Undertaken by Aviral Singh (Summer, Fall 2020).
5. "Rare-event simulations of CH_4 decomposition in Molten Tellurium"— Undertaken by Kanishka (Fall 2019).
4. "Modeling CH_4 to CH_3OH conversion in SSZ-13"— Undertaken by Anirban Ghosh (Fall 2019).
3. "Evaluating water force-fields in liquid phase using experimental radial distribution function"— Undertaken by Pranshu Tripathi (Fall 2018).
2. "Modeling CH_4 decomposition in Molten Tellurium"— Undertaken by Shivali Agrawal (Fall 2018).
1. "Evaluating water force-fields in gas-phase using accurate quantum chemical calculations" — Undertaken by Ashar Ahmad (Fall 2017).

Undergraduate Research Mentored (21)/Mentoring (3)

Anas Ali (SURGE, May'24–June'24); Akshat Mishra (SURGE, May'22-July'22); Vrahant Nagoria (May'21-Jun'22); Sunny Kumar Bhagat (SURGE, Feb'21-May'23); Ananyae Kumar Bhartari (Feb'21-current); Ayushi Goyal (SURGE, Jan'20–Dec'20); Aviral Singh (Mar'19–current); Anirban Ghosh (Mar'19–Nov'19); Kanishka (SURGE, Mar'19–current); Lakshyay Tyagi (June'19–July'19); Pranshu Tripathi (Dec'17–Dec'18); Shivali Agrawal(SURGE, Feb'18–Dec'18); Parth Chhaparwal (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)

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Course Instructor

Advanced Reaction Engineering (Fall 2022, Fall 2023, Fall 2024); Statistical Mechanics and Kinetics for Engineers (Fall 2020, Spring 2023); Chemical Engineering Thermodynamics (Summer 2019, Spring 2020, Spring 2021, Spring 2022); Practical Introduction to Quantum Chemical Methods (Spring 2018, Spring 2019. Spring 2024); Chemical Process Simulation Lab (Fall 2017, Fall 2018, Fall 2019).

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.

Funding

6. Core Research Grant, 2024 (∼61 lacs)
5. IRPHA, 2022 (∼8 crores)
4. Core Research Grant, 2022 (∼52 lacs)
3. Core Research Grant, 2019 (64.6 lacs)
2. IIT Kanpur, 2017 (25 lacs)
1. Ramanujan Fellowship, 2017 (38 lacs)