Vishal Agarwal

Associate Professor

107, Northern Laboratory II,
IIT Kanpur, Kanpur 208016,
Uttar Pradesh, India.

+91 (512) 259-6895

https://www.iitk.ac.in/che/va.htm

vagarwal@iitk.ac.in

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, 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 – Jan'24
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)

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 "Fundamentals of Chemical Reaction Engineering", 2025.
- Senate Chairman's Commendation for Tutoring "Thermodynamics", 2025.
- Senate Chairman's Commendation for Teaching "Chemical Reaction Engineering", 2024.
- 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.

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Interests

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Publications [hindex = 15; i10-index = 20]

44. Aditya Goyal, Horia Metiu*, and **Vishal Agarwal***, *Electrochemical Descriptors of the Catalytic Activity of Doped Molten Alkali Halide Salts for Methane Pyrolysis*, Journal of Physical Chemistry C, 130(14), 2026, 5115–5122.

43. Sandra Liz Simon, Nitin Kaistha*, and **Vishal Agarwal***, *An Active Learning Algorithm for Identifying Transition States on a Potential Energy Surface*, Journal of Chemical Theory and Computation, 22(6), 2026, 2972–2986.

42. Abir Lal Bose, Raghav Singh Thakur, Goutam Deo*, and **Vishal Agarwal***, *Promotional Effect of Molybdena for Non-Oxidative Propane Dehydrogenation Reaction over ZrO_2 Supported Vanadia Catalyst: A Combined Experimental and Theoretical Study*, Chemical Engineering Science, 2026, 123272.

41. Juhi Srivastava, Horia Metiu*, and **Vishal Agarwal***, *Vapor and Molten Mg-Based Catalysts for Methane Activation*, Journal of Physical Chemistry C, 130(2), 2026, 871-1124.

40. Michael Dongwook Byun, Juhi Srivastava, Rami Jubeili, **Vishal Agarwal**, and D.Chester Upham*, *Hydrogen Dissociation and Diffusion through Molten Metal Alloy Membranes*, Journal of Membrane Science, 2025, 125078.

39. Nikil Surya Rajaprabhu, Aditya Goyal, **Vishal Agarwal***, *Molten Catalytic Systems for CO_2-Free H_2 Production from CH_4: A Perspective from Ab Initio Simulations*, Materials, Devices and Systems for Sustainability, Springer, 2025, 61-73. (Book Chapter)

38. Genpei Cai, Nikil Surya RajaPrabu, Juhi Srivastava, Korbinian Lechner, Jorit Körber, Zhiyuan Zong, Kevin J. Smith, **Vishal Agarwal***, and David Chester Upham*, *A melt-based reaction pathway for CO_2 and CH_4 conversion to syngas and carbon using liquid In–Sn*, Journal of Catalysis, 2025, 116465.

37. Genpei Cai, Nikil Surya RajaPrabu, Juhi Srivastava, Kevin J. Smith, **Vishal Agarwal***, and D. Chester Upham*, *Surface and Catalytic Properties of Molten In–Sn and In–Ni for Methane Dry Reforming and Pyrolysis*, Journal of Physical Chemistry C 129 (30), 2025, 13615–13626.

36. Sandra Liz Simon, Nitin Kaistha*, **Vishal Agarwal***, *Accelerated Relaxation Engines for Optimizing to Minimum Energy Path*, Reaction Chemistry and Engineering 10(10), 2025, 2285-2299.

35. Aditya Goyal, Baljit Singh, Horia Metiu, **Vishal Agarwal***, *Rate enhancing role of molybdenum chloride in molten KCl for methane activation*, The Journal of Chemical Physics 162 (20), 2025, 204702.

34. Deepak Kumar Gorai, Horia Metiu*, **Vishal Agarwal***, *Theoretical Investigation of Solvated Electron Chemistry in Molten $CaCl_2$*, The Journal of Physical Chemistry C 129 (10), 2025, 4907–4914.

33. Nikil Surya R., Raju Kumar Gupta, **Vishal Agarwal***, *Modeling the role of Ta-dopant and co-catalytic water for activation of CO_2 on anatase $TiO_2(101)$*, Molecular Catalysis 570, 2025, 114642.

32. Kanishka Charakhwal, **Vishal Agarwal***, *Role of H_2O_2 as Oxidant and H_2O as Co-catalyst over Anatase-TiO_2 (101) for Conversion of Methane to Methanol*, ChemPhys Chem 2024, e202400708.

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.

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.

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Interests

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

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. (Book Chapter)
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. (Book Chapter)
18. Horia Metiu*, **Vishal Agarwal**, Henrik H. Kristoffersen, *The Role of Computations in Catalysis*, Reviews in Computational Chemistry 31, 2018, 171-196.(Book Chapter)
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. (Book Chapter)
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.

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

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.

Invited Talks

20. **Vishal Agarwal***, *Catalysts: The Invisible Heroes of Modern life & how Computers help design them.*, invited by Lakshya Science Foundation Programme (LSFP), IIT, Kanpur, July 2026.
19. **Vishal Agarwal***, *Computational Design of Novel Molten Catalysts for CO_2-Free Production of H_2 from Methane Pyrolysis*, invited by Industrial Technology Research Institute (ITRI), Hsinchu, Taiwan, June 2025.
18. **Vishal Agarwal***, *Computational Design of Novel Molten Catalysts for CO_2-Free Production of H_2 from Methane Pyrolysis*, invited in Taiwan International Conference on Catalysis (TICC), Hsinchu, Taiwan, June 2025.
17. **Vishal Agarwal***, *Theory Driven Design of Molten Catalysts*, invited in HPC Symposium, Indian Institute of Technology (IIT) Kanpur, India, April 2025.
16. **Vishal Agarwal***, *Novel Algorithms for Finding Transition States*, invited in Recent Advances in Modeling Rare Events (RARE): Methods and Applications, Khajuraho, Madhya Pradesh, India, March 2025.
15. **Vishal Agarwal***, *Novel Molten Catalysts For CO_2 free Production of H_2 from Methane Pyrolysis*, invited by Catalysis and Reaction Engineering Symposium (CARES), Indian Institute of Technology (IIT) Madras, India, September 2024.
14. **Vishal Agarwal***, *Novel Algorithms for Efficient Exploration of Potential Energy Surfaces*, invited in HPC Symposium, 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, February.2024.

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12. Krishna Jaiswal*, Horia Metiu, **Vishal Agarwal**, *Rates of Desorption on a Solid-Liquid Interface*, invited in Theoretical Chemistry Symposium (TCS), IISER Kolkata, India, December 2021.
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 in Advanced Simulation Methods (ASM), 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 (Contributed-Talks)

41. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *Novel Algorithms for Efficient Exploration of Potential Energy Surfaces*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2025.
40. Prateek Kumar Panday*, Swarnendu Biswas, **Vishal Agarwal**, *An Efficient Method for Computing Ewald Summation with 2D Periodicity*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2025.
39. Aditya Goyal*, Baljit Singh, Horia Metiu, **Vishal Agarwal**, *Ab initio molecular dynamics study to elucidate the role of Mo doping in molten KCl for methane activation*, UCRA3, Warsaw University of Technology, Warsaw, September 2024.
38. Nikil Surya R*, Genpei Cai, Juhi Srivastava, D. Chester Upham, **Vishal Agarwal**, *Dry reforming of methane in molten In-Sn alloy*, UCRA3, Warsaw University of Technology, Warsaw, September 2024. **(Second Prize)**
37. Nikil Surya R*, Raju Kumar Gupta, **Vishal Agarwal**, *Modeling the role of dopants and water on photocatalysis of CO_2,* Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, May 2024.
36. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *An Adaptive Acceleration Routine for Efficient MEP Discovery, Annual Meeting (AIChE)*, San Diego USA, October 2024.
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)**

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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.
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.

Vishal Agarwal

Associate Professor

107, Northern Laboratory II,
IIT Kanpur, Kanpur 208016,
Uttar Pradesh, India.

+91 (512) 259-6895

https://www.iitk.ac.in/che/va.htm

vagarwal@iitk.ac.in

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

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.
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.

Vishal Agarwal

Associate Professor

107, Northern Laboratory II,
IIT Kanpur, Kanpur 208016,
Uttar Pradesh, India.

+91 (512) 259-6895

https://www.iitk.ac.in/che/va.htm

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Interests

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

Conference Presentations (Posters)

38. Nikil Surya R*, Genpei Cai, Juhi Srivatsava, Abdul Kaish, Chester Upham, and **Vishal Agarwal**, *Dry Reforming of Methane on Molten In-Sn and In-Ni Alloys: Catalytic Activity and the Influence of Intermediate Carbon Species*, Faraday Discussion: Bridging the gap from surface science to heterogeneous catalysis, London, UK, April 2026.
37. Aditya Goyal*, Horia Metiu, and **Vishal Agarwal**, *Elucidating the Catalytic Activity of Molten Bismuth and Bismuth Trichloride Systems: A DFT Study*, Faraday Discussion: Bridging the gap from surface science to heterogeneous catalysis, London, UK, April 2026.
36. Siddharth Gautam*, Sandra Liz Simon, **Vishal Agarwal**, *A Novel Force-Based Mixing Method for Optimizing to Minimum Energy Path*, Workshop on accelerating scientific discovery in Chemistry and Material Science with HPC and AI (ACMS 2025) at HiPC 2025, Hyderabad, India, December 2025.
35. Siddharth Gautam*, Sandra Liz Simon, **Vishal Agarwal**, *A Novel Force-Based Mixing Method for Optimizing to Minimum Energy Path*, Workshop on accelerating scientific discovery in Chemistry and Material Science with HPC and AI (ACMS 2025) at HiPC 2025, Hyderabad, India, December 2025.
34. Prateek Kumar Pandey*, **Vishal Agarwal**, Swarnendu Biswas, *A Novel Method for Efficiently Computing Ewald Summation for Ionic Slab Geometries*, Workshop on accelerating scientific discovery in Chemistry and Material Science with HPC and AI (ACMS 2025) at HiPC 2025, Hyderabad, India, December 2025.
33. Sandra Liz Simon, Nitin Kaistha, **Vishal Agarwal***, *Novel Algorithms for Efficient Exploration of Potential Energy Surface,* 29^{th} *North American Catalysis Society Meeting (NAM29),* Atlanta, USA, June 2025.
32. Nikil Surya R, Genpei Cai, D. Chester Upham, **Vishal Agarwal***, *Role of carbon species in dry reforming and pyrolysis of methane: Insights from molten In-Sn and In-Ni alloys,* 29^{th} *North American Catalysis Society Meeting (NAM29),* Atlanta, USA, June 2025.
31. Prateek Kumar Panday*, Swarnendu Biswas, **Vishal Agarwal**, *An Efficient Method for Computing Ewald Summation with 2D Periodicity*, HPC symposium, IIT Kanpur, Uttar Pradesh, India, April 2025.
30. Juhi Srivastava*, Horia Metiu, **Vishal Agarwal**, *Theoretical Investigation of* CH_4 *Pyrolysis in Vapor and Molten Mg-based Catalysts*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2025.
29. Nikil Surya R*, Genpei Cai, D. Chester Upham, **Vishal Agarwal**, *Role of carbon species in dry reforming and pyrolysis of methane: Insights from molten In-Sn and In-Ni*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2025.
28. Aditya Goyal, Horia Metiu, **Vishal Agarwal***, *Elucidating the Catalytic Activity of Doped Molten Bismuth and Bismuth Trichloride Systems: A DFT Study*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2025.
27. Abir Lal Bose*, Raghav Singh Thakur, Goutam Deo, and **Vishal Agarwal**, *Molybdena as a promoter for propane dehydrogenation (PDH) reaction over* ZrO_2 *supported vanadia catalyst: An Experimental + DFT study*, HPC symposium, IIT Kanpur, Uttar Pradesh, India, April 2025.
26. Abir Lal Bose*, Raghav Singh Thakur, Goutam Deo, and **Vishal Agarwal**, *Molybdena as a promoter for propane dehydrogenation (PDH) reaction over* ZrO_2 *supported vanadia catalyst: An experimental+DFT study*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2025.
25. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *Adaptively Accelerated Strategies for Efficient MEP Discovery, Recent Advances in Modeling Rare Events (RARE)*, Khajuraho, Madhya Pradesh, India, March 2025.

Vishal Agarwal

Associate Professor

107, Northern Laboratory II,
IIT Kanpur, Kanpur 208016,
Uttar Pradesh, India.

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

24. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *Adaptive acceleration routines for efficient MEP discovery*, ACS Spring, San Diego USA, March 2025.
23. Abir Lal Bose*, Raghav Singh Thakur, Goutam Deo and **Vishal Agarwal**, *A combined experimental and theoretical approach to investigate the role of molybdenum oxide (Molybedena) as a promoter for propane dehydrogenation reaction over ZrO_2 supported vanadia catalyst*, CACEE 2024, TIFR Mumbai, Mumbai, December 2024.
22. Abir Lal Bose*, Sayali Ramteke, Goutam Deo and **Vishal Agarwal**, *A combined experimental and DFT study to investigate the role of molybdena as a promoter for propane dehydrogenation (PDH) reaction over ZrO_2 supported vanadia catalyst* Institute Research Symposium, IIT Kanpur, Uttar Pradesh, India, November 2024.
21. Abdul Kaish*, Juhi Srivastava, D.Chester Upham, **Vishal Agarwal**, *Activation of dry reforming of methane by In-Ni and In-Sn alloy*, IIChE-CHEMCON, Heritage Institute of Technology, Kolkata, December 2023.
20. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *Adaptively accelerated relaxation engine (AARE) for optimizing minimum energy path*, Theoretical Chemistry Symposium(TCS), IIT Madras, India, December 2023.
19. Abir Lal Bose*, Sayali Ramteke, Goutam Deo and **Vishal Agarwal**, *Modeling isolated monomeric MoO_x and VO_x clusters on ZrO_2 support and their interaction with each other: A DFT+U Study*, EuEuChems CompChem 2023, Thessaloniki, Greece, August 2023. (**Received International Travel Grant**)
18. Abir Lal Bose*, Sayali Ramteke, Goutam Deo and **Vishal Agarwal**, *A DFT+U study to model isolated monomeric MoO_x clusters on ZrO_2*, MSSAP, IIT Bombay, Maharashtra, India, June 2023. (**2nd best best poster award**)
17. Aditya Goyal*, and **Vishal Agarwal**, *Mechanistic modeling of keto-enol tautomerization reaction in Sn doped BEA zeolite*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2023.
16. Nikil Surya R*, Raju Kumar Gupta, **Vishal Agarwal**, *Modeling methane pyrolysis in molten sodium catalyst* , Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2023.
15. Nikil Surya R*, Raju Kumar Gupta, **Vishal Agarwal**, *Modeling the role of dopants and water on photocatalysis of CO_2*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2023.
14. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *Developing novel algorithms for finding minimum energy path*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2023.
13. Baljit Singh*, Sajal Kanti Dutta, Horia Metiu, and **Vishal Agarwal**, *Modeling the Surprise Increase in Activity of Molten Salts by Doping*, Research Scholars Day, IIT Kanpur, Uttar Pradesh, India, April 2023.
12. Sandra Liz Simon*, Nitin Kaistha, **Vishal Agarwal**, *Developing novel algorithms for exploring potential energy surfaces and reaction pathways*, Institute Research Symposium, IIT Kanpur, Uttar Pradesh, India, January 2023.
11. Aditya Goyal*, and **Vishal Agarwal**, *Mechanistic modeling of keto-enol tautomerization reaction in Sn doped BEA zeolite*, Institute Research Symposium, IIT Kanpur, Uttar Pradesh, India, January 2023.
10. 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*, Institute Research Symposium, IIT Kanpur, Uttar Pradesh, India, January 2023.
9. Fouziya Anjum*, Kanwar S Nalwa, **Vishal Agarwal**, *Investigating the effect of LiI on the decomposition of Li_2O_2*, Institute Research Symposium, IIT Kanpur, Uttar Pradesh, India, January 2023.
8. Abir Lal Bose*, Sayali Ramteke, Raghav Singh Thakur, Goutam Deo, and **Vishal Agarwal**, *A DFT+U study to model monomeric MoO_x and VO_x clusters supported on ZrO_2 and their interaction with each other* , Institute Research Symposium, IIT Kanpur, Uttar Pradesh, India, January 2023.

Vishal Agarwal

Associate Professor

107, Northern Laboratory II,
IIT Kanpur, Kanpur 208016,
Uttar Pradesh, India.

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https://www.iitk.ac.in/che/va.htm

vagarwal@iitk.ac.in

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

7. Aditya Goyal*, and **Vishal Agarwal**, *Modeling the role of water in Sn-BEA zeolite for Keto/enol tautomerization of acetone*, ICEC, Osaka, Japan, July 2022.
6. Abir Lal Bose*, and **Vishal Agarwal**, *A DFT+U study to model reduced MoO_x surfaces for hydrodeoxygenation of bio-oil model compounds*, ICEC, Osaka, Japan, July 2022.
5. Nikil Surya R*, Raju Kumar Gupta, **Vishal Agarwal**, *Modeling the role of water on photo-catalysis of CO_2*, SUNRISE: Transition to Net Zero, Swansea, UK, February 2022.
4. Sajal Kanti Dutta*, Smita Ghosh, Horia Metiu, **Vishal Agarwal**, *'Direct conversion of methane to hydrogen using gas-phase metal halides: DFT and microkinetic modeling*, SUNRISE: Transition to Net Zero, Swansea, UK, February 2022.
3. Sajal Kanti Dutta*, **Vishal Agarwal**, *'DFT study of phenol alkylation with propylene in H-β Zeolite*, ISCRE 26, New Delhi, India, December, 2021.
2. Sajal Kanti Dutta*, **Vishal Agarwal**, *'DFT study of bio-oil upgradation using H-beta zeolite*, SUNRISE: Energy Sustainability and Water, IIT Kanpur, Kanpur, Uttar Pradesh, India, February, 2021.
1. Krishna Jaiswal*, Jaishri Jain, Kumari Shilpa, **Vishal Agarwal**, *A Functional Force Field Model for Water Based on Gaussian charges*, MOLSIM, IIT Kanpur, Kanpur, Uttar Pradesh, India, February, 2020.

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 Catalysis, ACS Catalysis, Nature Communications, International Journal of Hydrogen Energy, Journal of Physical Chemistry, Langmuir, Catalysis Science & Technology, ACS Applied Energy Materials, Korean Journal of Chemical Engineering, Molecular Catalysis, ACS Engineering Au, Surfaces & Interfaces, Catalysis Letters, International Journal of Molecular Science, Environmental Science and Technology, ChemCatChem, Computational & Theoretical Chemistry, Reactor, Kinetics, Mechanisms & Catalysis, Journal of Chemical Sciences, Applied Physics Letters, Materials Science in Semiconductor Processing, Canadian Journal of Chemistry, Proceedings of the National Academy of Sciences, India Section A: Physical Sciences, 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).

Teaching and Mentoring

Phd Theses Supervised (3)/Supervising (3)

6. "Machine Learning Accelerated Solution for the Schrödinger Equation for Computational Chemistry Applications"— Undertaken by Siddharth Gautam (2024-current).
5. "Developing Novel Algorithms For Exploring Potential Energy Surfaces"— Undertaken by Sandra Liz Simon (co-supervised with Prof. Nitin Kaistha; 2021-current).

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4. "Engineering Biomass-Derived Porous Carbons for Enhanced CO_2 Capture"— Undertaken by Rupesh Singh (co-supervised with Prof. Raju Kumar Gupta; 2020-current).
3. "Modeling the Role of Dopant for Selective Catalytic Applications"— Undertaken by Aditya Goyal (2019-2025).
2. "Investigating the Nature of Active Sites in Doped-TiO_2 and Molten Catalysts for CO_2 and CH4 Activation"— Undertaken by Nikil Surya (co-supervised with Prof. Raju Kumar Gupta; 2019-2025).
1. "Predictive Modeling of Hydrodeoxygenation Catalyst for Biofuel Upgrading"— Undertaken by Abir Lal Bose (2018-2025).

Master's Theses/Project Supervised (15)/Supervising (2)

17. "Modelling the Growth of Carbon Nanotubes on Molten Cu-In droplet using Machine learning"— Undertaken by Anmol Bansal (2024-current).
16. "Molten Salt Catalysis for Methane Pyrolysis"— Undertaken by Jayant Mahlawat (co-supervised with Prof. Himanshu Sharma; 2024-current).
15. "Mechanistic Modelling of Methane Activation on Molten Cu-In Droplets"— Undertaken by B S Nishok Balaji (2024-2026).
14. "Designing Novel Algorithms for Parallelization of 2D EWALD Summation"— Undertaken by Prateek Kumar Panday (2023-2025); co-supervised with Prof. Swarnendu Biswas.
13. "Effect of Secondary Metaloxide on Oxidative Dehydrogenation of Propane over Vanadia Supported Zirconia Catalysts"— Undertaken by Subhadeep Dey (2022-2024); co-supervised with Prof. Goutam Deo.
12. "Modeling Molten In-Ni Alloy for Dry Reforming of Methane"— Undertaken by Abdul Kaish (2022-2024).
11. "CO_2-Free Methane Pyrolysis to H_2 in Molten KCl doped with $MoCl_5$ and Mo_2C"— Undertaken by Vikash Kumar Gupta (2022-2024); 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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Associate Professor

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PostDoctoral Fellows Supervised (5)/Supervising (1)

6. "Dry Reforming of CH_4 in Doped Molten Salts"— Undertaken by Dr. Nidhi Tiwari (2025-current).
5. "Modelling CH_4 Decomposition in Molten Mg and Mg-Zn Alloys"— Undertaken by Dr. Juhi Srivastava (2022-2025).
4. "Modelling the Chemistry of Solvated Electrons in Metal Doped Metal Halides"— Undertaken by Dr. Deepak Gorai (2023-2024).
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 (2019-2023).

Undergraduate Project Supervised (16)

16. "Developing Methods to Improve AL-NEB: An Active Learning Framework to Find Transition State"— Undertaken by Shreshth Gupta (Summer 2026).
15. "Implementation of a Machine-Learned Inter-atomic Potential (MLIP) for Molten Catalysis of Carbon Nanotubes"— Undertaken by Sourish Das (Summer 2026).
14. "Testing Accelerated Relaxation Engines for Optimizing to a Minimum Energy Path"— Undertaken by Asmi Katiyar (Summer 2026).
13. "Testing the Efficiency of Different Optimizer Algorithms (AARE and FIRE) for the Zinc Halide System"— Undertaken by Sanchit Singh (Summer 2025).
12. "Evaluating the Efficiency of Novel Algorithms for Transition State Identification in Methane Pyrolysis"— Undertaken by Karan Keer (Summer 2025).
11. "Exploring Activity of Gas Phase $CrCl_2$ for CH_4 Pyrolysis using Novel Optimization Techniques"— Undertaken by Anas Ali (Summer 2024).
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).

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vagarwal@iitk.ac.in

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

Undergraduate Research Mentored (28)/Mentoring (1)

Shreshth Gupta (SURGE, May'2026–July'2026), Asmi Katiyar (May'26–Jun'26), Krishana Yadav (May'26–July'26), Sanchit Singh (SURGE, May'25–July'25); Karan Keer (SURGE, May'25–July'25); Khushi Kumari (May'24–Dec'24), 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)

Course Instructor

Fundamentals of Chemical Reaction Engineering (Fall 2025, Fall 2026); Chemical Engineering Thermodynamics (Spring 2026); Chemical Process Simulation Lab (Summer 2025); Chemical Kinetics Reaction Rate Theories and Rare-event Simulations (Spring 2025); 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

Thermodynamics (Fall 2024, Fall 2025, Fall 2026) Computational Methods in Engineering (Fall 2017); Atoms, Photons and Molecules (Spring 2017).

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

7. Indo-Taiwan Research Grant, 2026 (∼46 lacs, PI)
6. Core Research Grant, 2024 (∼61 lacs, PI)
5. IRPHA, 2022 (∼8 crores, co-PI)
4. Core Research Grant, 2022 (∼52 lacs, co-PI)
3. Core Research Grant, 2019 (64.6 lacs, PI)
2. IIT Kanpur, 2017 (25 lacs, PI)
1. Ramanujan Fellowship, 2017 (38 lacs, PI)