

Curriculum Vitae

Jayant K. Singh, FNA, FASc, FNASc, FNAE
Om Prakash Gautam Chair Professor
Department of Chemical Engineering
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Education

Ph.D. Chemical and Biological Engineering, UB, SUNY at Buffalo 2004
M.S. Computer Science and Engineering, UB, SUNY at Buffalo 2002
B.Tech. Chemical Engineering, Indian Institute of Technology Kanpur 1997

Field of Specialization

- Gas separation & Storage (CO₂ capture)
- Drug, material and speciality chemical discovery
- Statistical mechanics, Thermodynamics, and molecular simulations
- Machine learning & AI based disruptive technologies

Awards and Honors

- Associate Editor, ACS J. Chemical Engineering Data 2026
- Elected Fellow, Indian National Science Academy 2026
- Om Prakash Gautam Faculty Chair Professor 2025
- Elected Fellow, Indian Academy of Sciences 2025
- Editorial Advisory Board Member, Advanced Intelligent Discovery 2024
- INAE-SERB Abdul Kalam Innovation National Fellowship 2023
- NASI-Reliance Industries Platinum Jubilee Award 2022
- STEM Impact Award (for Bhu-Parikshak) 2022
- Padma Bhushan Prof. L. K. Doraiswami CHEMCON Distinguished Speaker Award 2022
- Elected Fellow, Indian National Academy of Engineering 2022
- Herdillia Award, IChE 2021
- Elected Fellow, National Academy of Science, India 2021
- Poonam and Prabhu Goal Chair Professor 2021
- SERB-STAR Award 2020
- Editorial Board Member, Fluid Phase Equilibria 2020
- Editorial Advisory Board Member, J. Chemical Engineering Data 2020

- CSIR-CSMCRI Chemcon Distinguished Speaker Award 2019
- Editorial Advisory Board Member, ACS Omega 2018
- Mr. and Mrs. Gian Singh Bindra Chair Professor 2017
- JSPS Invitation Fellowship 2017
- Associate Editor, Chemical Engineering Communication 2016
- Guest Editor, Special Issue, Molecular Simulation 2014
- Class of 1970 Research Fellowship, IIT Kanpur 2013
- Member of Editorial Board, The Scientific World Journal 2012
- Humboldt Research Fellowship for Experienced Researchers 2012
- Elected as Member, National Academy of Sciences India (NASI) 2011
- Amar Dye-Chem Award, IChE 2010
- Indian National Academy of Engineering (INAE)
Young Engineer Award 2009
- DST-BOYSCAST Fellowship, DST 2008
- IIT Kanpur Reach Symposium Award 2007
- Research Fellow, Nanyang Technological University, Singapore 2007
- DAE-BRNS Young Scientist Award 2006
- New York State-GSEU Professional Development Award 2003

Experience

PIC Infra & Planning	December 2025-	Institute of Technology Kanpur
Chairman Oversight Committee	December 2024	Gangwal School of Medical School and Technology, IIT Kanpur
HAG Professor	August 2022-	Department of Chemical Engineering, IIT Kanpur
Head	January 2022-December 2024	Department of Chemical Engineering, IIT Kanpur
Member Founding Member	July 2021- Feb 2023	Chandrakanta Kesavan Center for Energy Policy and Climate Solutions
Adjunct Faculty & Founding Member	November 2020- June 2023	Department of Sustainable Energy Engineering, IIT Kanpur
Founder & Executive Director	June 2020-April 2022	IIT Kanpur Development Foundation (section 8 company)
Board member	July 2020-April 2022	IIT K Foundation, USA

Founder and Director	September 2019-	Prescience Insilico Pvt. Ltd.
Dean of Resources and Alumni	July 2019-March 2022	Institute of Technology Kanpur
Head, CCE/QIP	April 2018-June 2019	Institute of Technology Kanpur
Coordinator, HPC Centre	April 2015-Feb 2020	Institute of Technology Kanpur
Visiting Professor	June-July 2018; June 2019	Department of Physical Chemistry, Technical University Darmstadt, Germany
Visiting Professor	May 2017	Department of Chemistry, Okayama University, Japan
Nodal coordinator, National Super Computing	Sep 2016-Aug 2019	Institute of Technology Kanpur
Associate Dean of Academic Affairs	May 2016-July 2018	Institute of Technology Kanpur
Visiting Professor	June 2016	Department of Chemistry, University of Porto, Portugal
Visiting Professor	May 2016	Laboratory of Engineering Thermodynamics (LTD) University of Kaiserslautern
Visiting Professor	June-July 2015, June, 2016	Department of Physical Chemistry, Technical University Darmstadt, Germany
Professor	June 2015 – July 2022	Department of Chemical Engineering, Indian Institute of Technology, Kanpur, India
Visiting Professor	July 2012-June 2013; May-July 2014	Department of Physical Chemistry, Technical University Darmstadt, Germany
Associate Professor	Nov. 2010- June 2015	Department of Chemical Engineering, Indian Institute of Technology, Kanpur, India
Visiting Assistant Professor	May 2009 – Dec 2009	School of Chemical and Biomolecular Engineering, Vanderbilt University
Research Fellow	May 2007 – Jun 2007	School of Chemical and Biomedical Engineering, NTU, Singapore

Assistant Professor	Dec 2005-Nov 2010	Department of Chemical Engineering, Indian Institute of Technology, Kanpur, India
Research Scientist	Dec 2004-Nov 2005	General Motors India Science Lab, India
Research Intern	Jun 2002-Aug 2002	Buffalo Research Center, Honeywell Inc, USA
Research Scientist	Jun 2001-Dec 2001	CEDAR Tech, Amherst, NY
Research Scientist	May 1998-July 1999	Department of Chemical Engineering, IIT Kanpur
Process Engineer	May 1997-Apr 1998	Bechtel India

LIST OF PUBLICATIONS

(A) PATENTS

1. Jaiswal D, Bera JK and Singh JK, *Zr-Doped Ti_3C_2Tx MXene for CO_2 Utilization and Method of Preparation There of* (filed 2025)
2. Singh JK, Prince P, Ahmad A, Khan MA and Khemani Y, *Portable Smart Device for Determination of Soil Nutrients* (Granted, 2020)
 - a. Technology is transferred and licensed (for Indian Market) to **AgroNxt Pvt. Ltd.**
3. Singh JK, Singh P, Khan A, Rupaliya A and Kemani, Y, *Muhn Parikshak: Oral Cancer Testing Device.* (Granted, 2025)
 - a. Technology is transferred and licensed to **Scangenie Scientific Pvt. Ltd.**
4. Singh JK, Singh P, Khan A, Rupaliya A and Kemani, Y, *Karn Parikshak: Portable Otoscope for detection of various ear diseases.* (applied, 2024)
5. Singh JK, Srivastava P, Sahu CS, Srivastava A, Chand T and Kumar V, *A system for measuring nutrient in the soil and method thereof* (Patent number, 45992, granted 17/10/23)
6. Verma N, Singh JK and Sharma AK, *Polymeric nanocomposites and methods for their preparation and use*, US Patent: US Patent 20,150,267,011, 2015
 - a. **Technology transferred to Intellectual Ventures.**
7. Sharma AK, Singh JK and Verma N, *Preparation of activated carbon fibers/carbon nanofibers dispersed PVA nanocomposite material for lithium ion electrolyte battery separator* (Indian patent No: -IN-839267-01-IN-REG)

(B) BOOK

1. Singh JK and Verma N, *Aqueous Phase Adsorption: Theory, Simulations and Experiments*, CRC Press, ISBN 978-1138575219 (2019)

(C) OTHER BOOK AUTHORIZING ACTIVITIES

2. Book titled *Chemical Engineering Thermodynamics* by Kevin D. Dahm and Donald P. Visco, Jr, FPS system to SI units, Cengage Press, 2014

(D) CHAPTERS IN BOOKS

3. Bakinala M, Mullapudi, J and Singh, JK, MXenes for Electrochemical CO₂ Conversion: A DFT Perspective in the Age of MXenes: Prospects of 2D-Transition Metal Carbides and Nitride, ACS Book, in press, 2023
4. Katiyar P and Singh JK, The effect of nanoparticles on the oil-water interfacial tension in presence of nonionic surfactants in *Bijels, Bicontinuous particle-stabilized emulsions*, (Edited by Paul C. Clegg) RSC, ISBN 978-1-78801-520 (2020)
5. Singh JK, *Chemical Modeling of Fluids near Surfaces* in *Chemical Modeling*, vol. 8, 72-104, 2017, Royal Society of Chemistry
6. Patra TK, Khan S, Srivastava R and Singh, *Understanding wetting transitions using molecular simulations in Nanoscale and Microscale Phenomena*, Springer, 2015 (ISBN: 978-81-322-2289-7)
7. Khan S and Singh JK, *Molecular simulation of wetting transitions on novel materials* in *Molecular Modeling for the Design of Novel Chemicals and Materials*, Edited by B. Rai, CRC Press, 2012 (ISBN: 978-1439840788).
8. Singh SK and Singh JK, *Molecular modeling of capillary condensation in porous materials* in *Molecular Modeling for the Design of Novel Chemicals and Materials*, Edited by B. Rai, CRC Press, 2012 (ISBN: 978-1439840788).
9. Kwak SK and Singh JK, *Solid-liquid phase transition under confinement* in *Molecular Modeling for the Design of Novel Chemicals and Materials*, Edited by B. Rai, CRC Press, 2012 (ISBN: 978-1439840788).
10. Singh JK, Docherty H and Cummings PT, *Phase transition under confinement* in *Computational Nanoscience*, Edited by E. Bichoutskaia, Royal Society of Chemistry(RSC), 2011 (ISBN: 978-1849731331).
11. Singh JK, *Molecular Modeling and Simulation: Can it help in the development of micro and nano devices*, in *Microfluidics and Microfabrication*, S. Chakroborty (Ed), Springer (USA), 1st Edition 2009 (ISBN: 978-1441915429).

(E) IN REFEREED JOURNALS (204)

1. Rajpoot D, Srivastava D, Mir SH, Singh JK and Gopakumar TG, Unveiling the Effects of Nitrogen Doping and Stacking Sequences on the Electronic Structure of Imine-Based 2D Covalent Organic Frameworks, *Accepted Phys. Chem. Chem. Phys.* 2026
2. Chakraborti T, Sharma R, Krishnamoorthy A and Singh JK, Influence of microstructure on the dynamical properties of HMT-PMBI polymeric membrane: A molecular simulations study, *Accepted, ACS Applied Polymer Materials* 2026
3. Krishnan M, Vishwakarma, M, Tagad, A, and Singh JK, Unravelling Ice Growth Inhibition by UiO-66 and Its Functionalized Nanoparticles: The Role of Uncoordinated Linkers in Enhancing Interfacial Interactions with Ice, *Accepted, ACS Applied Materials and Interfaces*, 2026
4. Srivastava D, Mir SH, Singh JK and Gopakumar TG, Unveiling the effects of nitrogen doping and stacking sequence on the electronic structure of imine based 2D covalent organic frameworks. *Accepted ACS Applied Materials and Interfaces*, 2026
5. Jyothirmay MV et al, From Density Functional Theory to Machine Learning: Emerging Paradigms in Energy Materials Discovery, *Journal of Power Sources*, 671, 239478, 2026
6. Roy S and Singh JK: Heptazine-based g-C₃N₄-supported efficient single atom electrocatalysts for HER/OER/ORR: A first-principles study, *International Journal of Hydrogen*, 198, 152680, 2026
7. Upadhyay SN and Singh JK, Unveiling Atomic-Scale Mechanisms of Tantalum-Based 2D Materials for High-Performance Li–S Batteries, *Sustainable Energy & Fuels*, 8, 6733-6745, 2025
8. Krishnan M and Singh JK, Exploring cascaded adsorption cooling cycles with MOF – hydrocarbons integration: An accelerated approach using Bayesian Optimization and Monte Carlo Simulations, *Journal of Material Chemistry A*. 13, 38964-38977, 2025
9. Jaiswal D et al, Zirconium-Based MXene: A Novel Dual Functional Material for Integrated CO₂ Capture and Conversion, *Chemical Communications*, 61,17693-17696, 2025
10. Bind, S, Singh JK and Sharma H, Effect of Brine Composition on the Surface Energy of Calcite and Adhesion of Oil: Implications for the Wettability of Limestone Rocks, *Journal of Molecular Liquids*, 437, 128606, 2025
11. Bhendale M, Singh JK, Zacccone A, Shear Induced diffusivity in supercooled liquids *Journal of Chemical Physics*, 163, 144502, 2025

12. Sharma R, Chakraborti T and Singh JK, Understanding the role of Alkyl Chain Architecture and Functional Group Chemistry in governing Ion Transport in PEEK based Anion Exchange Membranes: A Molecular Dynamics Study, *J. Membrane Science*, 736, 124598, 2025.
13. Sharma R, Bhendele M, Das S, Mahapatra S and Singh JK et al, Morphological and Microstructural Insights into Mixed Surfactant Systems: A Molecular Dynamics Study, *Soft Matter*, 21, 7519-7534, 2025.
14. Daoo V and Singh JK, A Generalized Framework for Data-Efficient and Extrapolative Materials Discovery for Gas Separation, *Advanced Intelligent Discovery* (<https://doi.org/10.1002/aidi.202500109>) 2025.
15. Chakraborti T, Sharma R, Krishnamoorthy A and Singh JK, Influence of microstructure on the dynamical properties of HMT-PMBI polymeric membrane: A molecular simulations study, *Journal of Physical Chemistry C*, 129, 26, 12053-12067, 2025.
16. Upadhyay SN and Singh JK, Unraveling the Catalytic Potential of 2D Nb₂Se₂C for Lithium Polysulfide Conversion: A DFT Study, *ACS Applied Energy Materials*, 8, 6733-6745, 2025
17. Birla H, Mir S, Yadav, K, Halbritter T, Heckel A, Singh JK and Gopakumar TG, Unusual One-Dimensional Cascade Effect in the Thermal and Photo-Induced Switching of Azobenzene Derivatives on Graphite Surface, *Chemical Science*, 16, 6325-6335, 2025.
18. Krishnan MS and Singh, Can MOF-isobutane integration enhance adsorption refrigeration cycle? An accelerated approach using Active Learning and Monte Carlo Simulations, *Fluid Phase Equilibria*, 592, 114315, 2025
19. Jyothirmmai MV and Singh JK, Computational Insights into the Adsorption of Organic Compounds on Peptide Surfaces, *Surfaces and Interfaces*, 56, 105624, 2025
20. Bhendele M, Sharma R and Singh JK, Cosolvent Induced Phase Transitions in ABA Block Copolymers: A Molecular Dynamics Study, *Macromolecules*, 57, 11576-11585, 2024
21. Abraham B , Jyothirmmai MV, Sinha P and Singh JK, Machine Learning Driven Advancements in Catalysis for Predicting Hydrogen Evolution Reaction Activity, *Materials Chemistry and Physics*, 326, 129895, 2024
22. Krishnan SM, Sharma R, and Singh JK, Optimising Adsorption Refrigeration with MOF-propane integration: a Sustainable Approach, *Journal of Materials Chemistry A*, 12, 21200-21212, 2024
23. Abraham M et al *Catalysis in Digital Age: Unlocking the power of data using machine learning*, *WIRE Computational Molecular Science*, 14, e1730, 2024

24. Chakraborti T, Sharma R, Krishnamoorthy A and Singh JK, Unravelling the effect of molecular interactions on macroscale properties in Sustained AEM under hydrated conditions using MD simulations, *Journal of Membrane Science* 705, 122887, 2024
25. Aqib M, Daoo V and Singh JK, Efficient Xylene Isomer Separation: Accelerated Screening with Active Learning and Molecular Simulation, *Energy & Fuels* 38, 9381-9394, 2024
26. Shrivastava D, Mishra V, Mir H Showkat, Dey J, Singh JK, Chandra M and Gopakumar G, Large Area Film of Highly Crystalline, Cleavable, and Transferable Semi-Conducting 2D-imine Covalent Organic Framework on Dielectric Glass Substrate, *ACS Applied Materials and Interfaces*, 16, 30485-30495, 2024
27. Jyothirmay MV, et al, Machine Learning Driven High-Throughput Screening of Transition Metal Atom Intercalated g-C₃N₄/MX₂ (M = Mo, W; X = S, Se, Te) Heterostructures for Hydrogen Evolution Reaction, *ACS Applied Materials and Interfaces*, 16, 12437-12445, 2024
28. Daoo V and Singh JK, Accelerating Insilico discovery of Metal-Organic Frameworks for ethane/ethylene and propane/propylene separation: A Synergistic Approach Integrating Molecular simulation, Machine learning, and Active learning, *ACS Applied Materials and Interfaces*, 16, 6971-6987, 2024.
29. Athawale A, Abraham B, Jyothirmay MV and Singh JK, MXene-Based Single Atom Catalysts for Electrochemical Reduction of CO₂ to Hydrocarbon Fuels, *Journal of Physical Chemistry C*, 127, 24542-24551, 2023.
30. Bhendele M, Indra A, Singh JK, Does freezing induces self-assembly of polymers? A molecular dynamics study, *Soft Matter*, 19, 7570-7579, 2023.
31. Parey V, Abraham B, and Singh JK, Surface Hydroxylation Mechanism of Zr₂X(OH)₂ (X = C, N, or B) MXenes: A Promising Catalyst for CO₂ Conversion into Formic Acid. *Materials Chemistry and Physics*, 310, 128444, 2023.
32. Gupta M, Daoo V and Singh JK, Amine decorated MOF for direct capture for CO₂ from ambient air, *Dalton Transaction*, 52, 11621-11630, 2023.
33. Indra A, Bhendele M and Singh JK, Understanding the role of polymers on the nucleation behaviour of water in dilute supercooled solutions, *Journal of Chemical Physics*, 159, 044502, 2023.
34. Srirangam S, Bhendele M and Singh JK, Is Universal Shear Behavior of supercooled water retained at higher pressures, *Physical Chemistry Chemical Physics*, 2023.
35. Abraham B, et al, Integrating Machine Learning and Molecular Simulation for material design and discovery, *INAE letters*, , 2023.

36. Birla H, Mir S, Khushboo Y, Halbritter T, Heckel A, Singh JK and Gopakumar T, Tuning the switching probability of azobenzene derivatives on graphite surface through chemical functions, *Journal of Physical Chemistry C*, 2023.
37. Tiwari S and Singh JK, Effect of monovalent and divalent salts on the interfacial and structural properties of vapor-liquid water interface in presence of sodium dodecyl sulfate, *Journal of Molecular Liquids*, 2023.
38. Abraham M et al Machine learning-driven discovery of key descriptors for CO₂ activation over two-dimensional transition metal carbides and nitrides, *ACS Applied Materials and Interfaces*, 15, 30117-30126, 2023.
39. Jyothimai D, Roshni M. V. Abraham M and Singh JK, Accelerating the Discovery of g-C₃N₄ Supported Single Atoms Catalysts for Evolution Reaction: A Combined DFT and Machine Learning Strategy, *ACS Applied Energy Materials*, 10, 5598-5606, 2023.
40. Bhendle M and Singh JK, Molecular insights on morphology and composition of mixed micelles formed by ionic surfactant and nonionic block copolymer in water using coarse-grained molecular dynamics simulations, *Langmuir*, 39, 5031-5040, 2023.
41. Abraham B, Sinha P, Halder P and Singh JK, Fusing Machine learning strategy with density functional theory to hasten the discovery of 2D MXene based catalysts for Hydrogen Evolution Reaction, *J. Mat. Chem. A*, 11, 8091-8100, 2023.
42. Halder P and Singh JK, Screening of Hypothetical Metal Organic Frameworks for Xylene Isomers and Ethylbenzene Separation, *Energy & Fuels*, 37, 2230-2236, 2023.
43. Khushbook Y, Birla H, Mir S, Halbritter T, Hecket A, Singh JK, Gopakumar T, Meta-stable initial condition for improving the switching probability in azobenzene derivative on surface, *Applied Surface Science*, 612, 155747, 2023.
44. Mir SH, Yadav VK and Singh JK, Efficient CO₂ capture and activation on novel two-dimension metal borides, *ACS Applied Material Interfaces*, 14, 29703-29710, 2022.
45. Jyothimai MV, Abraham BM and Singh JK, Pressure induced phase diagram of double-layer ice under confinement: A first-principles study, *Physical Chemistry Chemical Physics*, 24, 16647-16654, 2022.
46. Bhendle M, Srivastava A and Singh JK, Insights into the thermodynamics and morphology of different phases of pluronic L64 from molecular simulations using derived coarse-grained model, *Journal of Physical Chemistry B*, 126, 4731-4744, 2022.

47. Tewari S, Namsani S and Singh JK, Effect of salt on the adsorption of ionic surfactant at the air-water interface, *Journal of Molecular Liquid*, 360,119498, 2022.
48. Pramanik D, Pawar A, Roy S and Singh JK, Mechanistic insights of key host proteins and repurposed inhibitors regulating SARS- CoV-2 pathway. *Journal of Computational Chemistry*, 43, 1237-1250, 2022.
49. Abraham BM, Parey V and Singh JK, A strategic review of MXenes as emergent building blocks for future two-dimensional materials: Recent progress and perspectives, *Journal Material Chemistry C*, 10, 4096-4123, 2022.
50. Parey V, Abraham BM, Jyothirmai and Singh JK, Mechanistic Insights for Electrochemical Reduction of CO₂ into Hydrocarbon Fuels over O-Terminated MXenes, *Catalysis Science and Technology*, 12,2223-2231, 2022.
51. Kumawat A, Namsani S, Pramanik D and Singh JK Integrated docking and enhanced sampling based selection of repurposing drugs for SARS-CoV-2 by targeting host dependent factors, *Journal of Biomolecular Structure and Dynamics*, 40, 9897-9908, 2022.
52. Namsani S, Praminik D, Khan MA, Roy S and Singh JK, Metadynamics-Based Enhanced Sampling Protocol for Virtual Screening: Case Study for 3CLpro protein for SARS-COV-2. *Journal of Biomolecular Structure and Dynamics*, 40, 7002-7017, 2022.
53. Abraham BM, Singh JK, Tuning the structural properties and chemical activities of graphene and hexagonal boron nitride for efficient adsorption of steroidal pollutants, *Applied Surface Science*, 580, 152110, 2022.
54. K Suraj, Goswami A, Singh JK, Salt-Water System under Diamond Confinement, *Journal of Physical Chemistry C*, 125, 22283-22294, 2021.
55. Tewari S, Abraham BM, Singh JK, Insight into the mechanism of nanoparticle induced suppression of interfacial tension, *Journal of Molecular Liquid*, 339, 117177, 2021.
56. Goswami A and Singh JK, Homogeneous Nucleation of Sheared Liquids: Advances and Insights from Simulations and Theory, *Physical Chemistry Chemical Physics*, 23, 15402-15419, 2021.
57. Goswami A, Dalal IS, Singh JK, Universal Nucleation Behavior of Sheared Systems, *Physical Review Letters*, 126, 195702, 2021
58. Parey V, Abraham BM, Mir S and Singh JK High-throughput screening of atomic defects in MXenes for CO₂ capture, activation and dissociation, *ACS Applied Materials & Interfaces*, 13, 35585-35594, 2021.

59. Dutta P, Pramanik D and Singh JK, On the phase behaviour of pure PSPC and PEGylated multi-component lipid and their interaction with Paclitaxel: An all-atom MD study, *Langmuir*, 37, 10259-10271, 2021.
60. Goswami A and Singh JK, A Hybrid Topological and Shape-Matching Approach for Structure Analysis, *Journal of Chemical Physics*, 154, 154502, 2021.
61. Maurya M, Singh JK and Saito S, Effects of Interfaces on Structure and Dynamics of Water Droplets on a Graphene Surface: A Molecular Dynamics Study. *Journal of Chemical Physics*, 154, 164704, 2021.
62. Halder P, Prerna, Singh JK, Building Unit Extractor for Metal-Organic Frameworks, *Journal of Chemical Information and Modeling*, 61, 5827-5840, 2021
63. Halder P and Singh JK, High Throughput Screening of Metal-Organic Frameworks for Ethane-Ethylene Separation Using Machine Learning Technique. *Energy & Fuels*, 34, 14591-14597, 2020.
64. Goswami A, Dalal IS and Singh JK, Seeding Method for Ice Nucleation under Shear. *Journal of Chemical Physics*, 153, 094502, 2020
65. Yadav VK, Mir S, Mishra V, Gopakumar TG and Singh JK, A simple Molecular Design for Tunable Two-Dimensional Imine Covalent Organic Frameworks for Optoelectronic Applications. *Physical Chemistry Chemical Physical*, 22, 21360-21368, 2020
66. Misra V, Mir S, Singh JK and Gopakumar TG, Rationally Designed Semi-Conducting 2D Surface Confined Metal Organic Network. *ACS Applied Materials & Interfaces*, 12, 51122-51132, 2020
67. Maurya M and Singh JK, Selective separation of CO₂ from flue gas using carbon and boron nitride nanotubes as a membrane, *Energy & Fuels*, 34, 7223-7231, 2020
68. Mir S, Yadav VK and Singh JK, Recent advances in the carrier mobility of two-dimensional materials: a theoretical perspective. *ACS Omega*, 5, 14203-14211, 2020
69. Mir SH, Yadav VK and Singh JK, Electronic properties and superior CO₂ capture selectivity of metal nitride (XN) and phosphide (XP) (X = Al, Ga and In) sheets, *Applied Surface Science*, 527, 146445, 2020.
70. Singh P, Verma JK and Singh JK, Evaluation of salivary biomarkers for the detection of oral squamous cell carcinoma in an Indian population. *Nature Scientific Report*, 10, 7365, 2020
71. Bhangari RS, Yadav VK, Singh JK and Sinha N, "Functionalized Boron Nitride Nanosheets as Novel Adsorbents for Removal of Arsenic(III) from Contaminated Water. 5, 10301-10314, *ACS Omega*

72. Goswami R, Goswami A and Singh JK, d-SEAMS: Deferred structural elucidation analysis for molecular simulations, *Journal of Chemical Information and Modeling*, 60, 2169-2177, 2020.
73. Kommu A and Singh JK, A review on graphene-based materials for removal of toxic pollutants from wastewater, *Soft Materials*, 18, 297-322, 2020 (**Invited Article**).
74. Goswami A and Singh JK, Exploring the anomalous phase behaviour of high-pressure ices in diamond confinement, *Journal of Physical Chemistry C*, 124, 5460-5468, 2020.
75. Goswami A and Singh JK, A general topological network criterion for exploring the structure of icy nanoribbons and monolayers, *Physical Chemistry Chemical Physics*, 22, 3800-3808, 2020.
76. Saha P, Yadav V, Gurunaryanan V, Ramapanicker R, Singh JK, Gopakumar T, Revealing the limits of intermolecular interactions: Molecular rings of ferrocene derivatives on graphite surface, *Journal of Physical Chemistry Letters*, 11, 297-302, 2020.
77. Mishra S, Singh AK and Singh JK, Ferrous sulfide and carboxyl-functionalized ferroferric oxide incorporated PVDF-based nanocomposite membranes for simultaneous removal of highly toxic heavy-metal ions from industrial ground water, *Journal of Membrane Science*, 593, 117422, 2020.
78. Sappidi P and Singh JK, Molecular dynamics study on the adsorption of UO_2^{2+} from an aqueous Phase: Effect of grafting dibenzo crown ether and dicyclohexano crown ether on the polystyrene surface, *Journal of Chemical Engineering Data*, 65, 3, 1051-1059, 2020 (**Invited Article**).
79. Mir SH, Yadav VK and Singh JK, Computational study of the effect of functional groups on water adsorption in mesoporous carbons: Implications for gas adsorption, *Journal of Physics and Chemistry of Solids*, 136, 109156, 2020.
80. Mir SH, Yadav VK and Singh JK, Unraveling the stacking effect and stability in nanocrystalline antimony through DFT, *ACS Applied Nano Materials*, 2, 7103-7113, 2019.
81. Saha P, Yadav, Gurunaryanan, Ramapanicker R, Singh JK and Gopakumar TG, Understanding the adsorption energetics of growth polymorphs of ferrocene derivatives: Microscopic thermal desorption analysis, *Journal of Physical Chemistry C*, 123, 18488-18494, 2019.
82. Prerna, Goswami R, Metya AK and Singh JK, Study of ice nucleation on silver iodide surface with defects, *Molecular Physics*, 117, 3651-3663, 2019 (**Invited Article**).

83. Mishra V, Yadav V, Singh JK and Gopakumar TG, Electronic structure of a semi-conducting imine-covalent organic framework, *Chemistry-An Asian Journal*, 14, 4645-4660, 2019.
84. Yadav VK, Mir SH and Singh JK, A computational study of structural, electronic and carrier mobility of boron and phosphorus/nitrogen co-doped graphene, *Physical B: Condensed Matter*, 571, 291-295, 2019.
85. Bhangari RS, Singh AK, Namsani S, Singh JK and Sinha N, Magnetite coated boron nitride nanosheets for the removal of arsenic (V) from water, *ACS Applied Materials & Interfaces*, 11, 19017-19028, 2019.
86. Sappidi P, Boda A, Ali SK and Singh JK, Adsorption of gadolinium (Gd³⁺) ions on the di benzo crown ether (DBCE) and di cyclo hexano crown ether (DCHCE) grafted on the polystyrene surface: Insights from all-atom molecular dynamics simulations and experiments, *Journal of Physical Chemistry C*, 123, 12276-12285, 2019.
87. Singh AK, Mishra S and Singh JK, Underwater superoleophobic biomaterials based on waste potato peels for simultaneous separation of oil/water mixtures and dye adsorption, *Cellulose*, 26, 5497-5511, 2019.
88. Maurya M and Singh JK, Effect of ionic liquid impregnation in highly water stable MOFs, COFs and carbon-based adsorbents for post-combustion flue gas treatment, *Energy & Fuels*, 33, 3421-3428, 2019.
89. Yadav VK, Mir SH and Singh JK, Density functional theory study of aspirin adsorption on BCN sheets and their hydrogen evolution reaction activity: a comparative study with graphene and hexagonal boron nitride, *ChemPhysChem*, 20, 1-9, 2019.
90. Singh AK and Singh JK, An efficient use of waste PE for hydrophobic surface coating and its application on cotton fibers for oil-water separator, *Progress in Organic Coatings*, 131, 301-310, 2019.
91. Katiyar P and Singh JK, Evaporation induced self-assembly of different shapes and sizes of nanoparticles: A molecular dynamics study, *Journal of Chemical Physics*, 150, 044708, 2019.
92. Mir SH, Yadav VK and Singh JK, Boron-carbon-nitride sheet as a novel surface for biological applications: insights from density functional theory, *ACS Omega*, 4, 3732-3738, 2019.
93. Ghosh S and Singh JK, Hydrogen adsorption in pyridine bridged porphyrin-covalent organic framework, *International Journal of Hydrogen Energy*, 44, 1782-1796, 2019.

94. Metya AK and Singh JK, Ice adhesion mechanism on lubricant-impregnated surfaces using molecular dynamics simulations, *Molecular Simulation*, 45, 394-402, 2019.
95. Sappidi P, Mir SH and Singh JK, Effect of polystyrene length for the extraction of Gd^{3+} and UO_2^{2+} ions using dicyclohexano crown ether (DCH18C6) with octanol and nitrobenzene: A molecular dynamics study, *Journal of Molecular Liquids*, 271, 166-174, 2018.
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204. Singh J and Sharma A, Self organization in thin liquid films: Dynamics and patterns in system displaying a secondary minimum, *Journal of Adhesion Science and Technology*, **14**, 145-166, 2000.

(F) INVITED TALKS

1. Singh JK, Accelerating material discovery: integrating AI/ML and molecular simulations, IIT Jammu , March 18, 2026
2. Singh JK, Accelerating material discovery: integrating AI/ML and molecular simulations, INSA, Delhi , December 4, 2025
3. Singh JK, Accelerating Discovering 2D Materials for Sustainable Technologies, HUST, China, November 24, 2025
4. Singh JK, Digital R&D: Prospects & Challenges, TRIPS, Kanpur, August 21, 2025
5. Singh JK, *Machine learning and molecular simulation integrated approach for material design and discovery*, BITS Pilani at GOA campus, July 29, 2025.
6. Singh JK, *Machine learning and molecular simulation integrated approach for material design and discovery*, BASF India, Mumbai, Feb 28, 2024.
7. Singh JK, Supercooled water in the presence of nanostructured surface and under shear flow, ICMS, Taiwan, October 5-9, 2023
8. Singh JK, Decoding the Chemistry of 2D MXenes for CO₂ Capture and Conversion Through Machine Learning, CEES, IIT Mandi, September, 26, 2023
9. Singh JK, Insight into ice formation at extreme confinement and under shear flow, Department of Physical Chemistry, University of Barcelona, May 26, 2022.
10. Singh JK, Nuclear under shear flow, INAE annual convention, December 14-16, 2022.
11. Singh JK, New Insight into the ice formation: extreme confinement & under shear flow, IIT Bombay, January 2022.
12. Singh JK, New Insight into the ice formation: extreme confinement & under shear flow, Theoretical Chemistry Symposium, December 11-14, 2021.
13. Singh JK, Integrating traditional drug-screening approaches with molecular simulations: A COVID-19 case study, Webinar meeting on Complex fluid, complex flow and COVID-19, June 20, 2020.
14. Singh JK, Fundamentals of Wetting Transitions, Hindustan Unilever Ltd, April 15, 2020
15. Singh JK, Novel computational tool development for unearthing ice phase in confinement to material discovery for gas separations to automated drug screening, Dr. Reddy Institute of Life Science, Hyderabad, February 25, 2020
16. Singh JK, Unraveling nanoconfined world using molecular simulations, December 6, COMFLU-2019

17. Singh JK, What nanoparticles can do to bulk and interfacial properties? University of Crete, Greece, May 29, 2019
18. Singh JK, Insights into material behavior via molecular simulations, *Invictus Oncology Pvt. Ltd.* Delhi, October 24, 2018
19. Singh JK, *Fourth industrial revolution*, LEAP, IIT Kanpur, November 20, 2018
20. Singh JK, *Ice nucleation in presence of foreign substances*, Department of Chemistry, TU Darmstadt, June 12, 2018
21. Singh JK, *Ice nucleation in presence of foreign substances*, Department of Chemical and Biological Engineering, NUS, May 21, 2018
22. Singh JK, *Multi-scale simulations of energy materials: some case studies*, Shell India, R&D, April 12, 2018
23. Singh JK, *Phonon thermal transport in β -Cu₂Se using an ab initio derived force-field*, Discussion Meeting on Recent Advances in Molecular Simulations, IISc Bangalore, February 08-11, 2018
24. Singh JK, *Changing world of chemical engineering*, Ujjain Engineering College, 24 March, 2018
25. Singh JK, *Changing world of chemical engineering*, Madan Mohan Malaviya University of Technology, Gorakhpur, February 11, 2018
26. Singh JK, *Molecular insight into nucleation behavior of supercooled water on surfaces*. IMS, Japan, May 18, 2017
27. Singh JK, *What we can learn about nucleation of supercooled water on surfaces using molecular simulation ?* Okayama University, May 15, 2017
28. Singh JK, *Nanoparticles aggregation and dispersion behaviour, and its effect on thermophysical properties*, Jilin University, October 27, 2016
29. Singh JK, *Molecular insight into fluid behavior near substrate*, Univ Porto, Porto, June 28, 2016
30. Singh JK, *Understanding ice nucleation on nanostructured surfaces*, TU Darmstadt, June 19, 2016
31. Singh JK, *Understanding water behavior on soft/hard surfaces using molecular simulations*, TU Kaiserslautern, May 17, 2016
32. Singh JK, *Molecular insight into fluid behavior near substrate*, IISc Bangalore, April 7, 2016

33. Namsani S and Singh JK, *Dewetting dynamics of gold film on graphene: Implications for nanoparticle formation*, Faraday Discussion on Nanoparticle Assembly: From Fundamentals to Applications, IIT Mumbai, Feb 6-9, 2016
34. Singh JK, *Understanding the formation of Janus particles from nano droplets of alkyl thiols*, Tutzing, Germany, October 21, 2015
35. Singh JK, *Understanding the behavior of supercooled liquid in presence of surfaces using molecular simulations*, Institute of Thermodynamics, Univ. Stuttgart, Germany, July 07, 2015
36. Singh JK, *Understanding water(ice)-surface behavior*, Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung (IFAM), Bremen, Germany, June 25, 2015
37. Singh JK, *Coarse-grained molecular simulations of nanoparticles and nanocomposites*, BARC, January 16, 2015
38. Singh JK, *Oscillatory behavior of melting behavior of nanoconfined fluids*, TCS 2014, NCL Pune, December 18, 2014
39. Singh JK, *Solid-liquid transition of nanoconfined fluids*, TU Kaiserslautern, Germany, July 15, 2014
40. Singh JK, *Phase transitions of nanoconfined fluids*, SN Bose Institute Kolkatta, April 11, 2014
41. Singh JK, *Understanding supercooled liquid on nanostructured rough surfaces: A molecular dynamics study*, Max Plank Institute, Institute of Physics for Complex Fluids, Dresden, Germany , Feb 19, 2013
42. Singh JK, *Understanding phase transition at nanoscale: role of external field*, Univ at Porto, 04 December, 2012
43. Singh JK, *Cross over behavior of confined fluids: 3D to 2D*, TU Darmstadt, Germany, July 19, 2012
44. Singh JK, *Phase transitions at nanoscale: role of confinement*, TU Darmstadt, Germany, July 19, 2012
45. Singh JK, *Unveiling thermodynamics at nanoscale*. Planetary Lecture, IChE Annual Meeting, Annamalai University, December, 2010.
46. Singh JK, *Fluid near surfaces*, Department of Polymer Engineering, BITS Ranchi, January 29, 2010.
47. Singh JK, *Fluid near surfaces*, Department of chemical and biomolecular engineering, Vanderbilt University, November 23, USA, 2009.

48. Singh JK, *Molecular modeling and simulation of fluids near surfaces*, Modeling and simulation of chemical processes, HBTI Kanpur, February, 2009.
49. Singh JK, *Molecular modeling and simulation: Can it help in the development of micro and nano devices?*, INDO- US Workshop, IIT Kharagpur, 2009.
50. Singh JK, *Molecular simulation of fluids near surfaces*, HPC workshop, IISc Bangalore, November 2008.
51. Singh JK, *Fluids near surfaces*, Department of Mechanical Engineering, IIT Kanpur, September 2008.
52. Singh JK, *Multi-scale simulation of cluster formation and self Assembly*, Indo-US workshop, IIT Kanpur , 2007.
53. Singh JK, *Advanced methods for calculating cluster integrals and interfacial properties*, Department of Chemical Engineering, IIT Delhi, 2004.
54. Singh JK, *Advanced methods for calculating cluster integrals and interfacial properties*, Department of Chemical Engineering, IIT Kanpur, 2004.

(G) CONFERENCE PRESENTATIONS (Over 120 international and national talks and posters)

RESEARCH SUPERVISION

(A) Ph. D. Thesis

1. Varad Jayant Dao on “Data Driven Discovery of Metal Organic Frameworks for Gas Separation and Storage” 2026
2. Mangesh Bhendale on “ Understanding the macromolecular self-assembly and aggregation thermodynamics in polymer/surfactant solutions using multi-scale simulations” 2024
3. Shubham Tewari on “ Influence of nanoparticles and inorganic salts on the adsorption dynamics, structural and thermodynamic properties” 2023
4. Prosun Halder on “ Metal-organic frameworks design and screening for separation of hydrocarbons using molecular simulations and machine learning” 2022
5. Amrita Goswami on “ Crystal nucleation: challenges and future horizons under confinement and shear” 2021
6. Prasad Sonar on “Granular flows over rigid inclined bases that are either spring-supported or externally vibrated” 2019
7. Manish Maurya on “Molecular Simulation Studies on Selective Separation of CO₂/SO₂ from Flue Gas using Porous Materials” 2019
8. Parul Katiyar on “Behavior of nanoparticles at interfaces: structure, dynamics and thermodynamic properties” 2018
9. Atanu K. Metya on “Molecular Simulations of Ice Nucleation in the Presence of Foreign Substance” 2018
10. Anitha Kommu on “Removal of Heavy Metal ions and Organic Pollutants from Industrial Wastewater using Nanomaterials” 2017
11. N. Sadanandam on “Force field development and prediction of thermal conductivity of nanocomposites” 2017
12. Debdeep Bhandary “Understanding of Self-Assembled Monolayer using Molecular Dynamics Simulations” 2016
13. Ashish Bhateja on “Segregation of granular material: Theory, Experiments and Simulations” 2014
14. Tarak Patra on “Coarse grain molecular modeling of nanoparticle-polymeric system” 2014
15. Chandan Das on “Study of the effects of confinement on melting transition of Lennard-Jones and dipolar fluids” 2014
16. Sandip Khan. on “Wetting transition on patterned surface applications towards nanofluids” 2012
17. Pratima Gazbiyein on “Development of direct alkaline alcohol fuel cell” 2012
18. Sudhir K. Singh on “Phase equilibria and interfacial properties of confined fluids” 2010

(B) M.Tech Thesis

1. Vasamsetty Subhasree Navya, Understanding Generative Model Performance in Property-Guided Surfactant Design: A Deep Learning and Molecular Dynamics Study 2026

2. Bhumesh Panchal on “Understanding Ice Recrystallisation Inhibition by MOF linkers: A Machine Learning and Molecular Dynamics study” 2025
3. Surabhi Sharma on “ Understanding and Enhancing Soil Micronutrients Detection Through Spectroscopic and Machine Learning Methods“ 2025
4. Abhay Gupta on “ Detection of Ear Diseases using Deep Learning Approaches” 2024
5. Rupareliya Abhaykumar Ashvinbhai on “Oral Cancer Detection using ML/AI Approach” 2024
6. Vipin Kumar on “ Wettability Alteration due to Low Salinity Waterflooding in Carbonate Reservoir: A Molecular Dynamics Study” 2024
7. Dantuluri Roshini on “A Combined Density Functional Theory and Machine Learning Aided Screening of g-C₃N₄ Based Single Atom Catalysts for Hydrogen Evolution Reaction” 2023
8. Aindrila Indira on “Understanding the Role of Polymers on the Nucleating Behaviour of Water in Dilute Supercooled Solutions” 2023
9. Priyanka Sinha on “Accelerating the Discovery of 2D Mxenes for Hydrogen Generation using Machine Learning” 2023
10. Ajinkya S Athawale on “Electrochemical Reduction of CO₂ to CH₄ Using Mxene based single atom catalysis” 2023
11. Bavita Kumari on “The role of salts in the recovery of oil: a molecular simulation study” 2022
12. Snehitha Srirangam on “Effect of pressure on ice nucleation under shear” 2022
13. Jaysree Lakela on “Screening of hypothetical zeolites for the separation of hydrogen isotopes” 2022
14. Suraj K on “ Study of confined salt-water at gigapascal high pressure” 2021
15. Soumyadeb Ghosh on “ Study on the effect of combination of monovalent and divalent salts on interfacial tension at water-oil system in presence of surfactant” 2021
16. Ashar Ahmad on “Development of a rapid soil testing tool for real time sensing of soil physical and chemical properties” 2020
17. Prantar Dutta on “Drug-Lipid Interactions in Multicomponent Membranes: Insights from Molecular Dynamics Simulations” 2020
18. Tekchand Kumawat on “Development of a portable device for simultaneous determination of soil nutrients” 2019
19. Prerna on “Study of Ice Nucleation on Defective Silver Iodide and Effect of Probing on Dynamics of a Water Droplet” 2019
20. Ankit Srivastava on “Development of a sol-gel membrane for sensing nitrate ions” 2018
21. Sauradeep Majumdar on “Adsorptive Separation of CO₂ from Multicomponent Gas Mixtures in Nanoporous Materials” 2018
22. Chandra Sekhar Sahu on “Development of Handheld Device for Measurement of Micro and Macro Nutrients Concentration in Soil” 2018
23. Kumar Ketan on “Simple and green fabrication of recyclable highly hydrophobic/superoleophilic magnetic sorbents and filter paper for removal of oils and organic solvents from water” 2017

24. Sandip Charan on “ A Molecular Simulation Study of CO₂ Adsorption using Functionalized and Non- Functionalized CNTs” 2016
25. Naveen Rangera on “Effect of Different Surfactants on the Interfacial Behavior of n-Hexane-Water System in Presence of Silica, Titania and ZnO Nanoparticles” 2016
26. Prasun Haldar on “Selective adsorption of CO₂ using functionalized CMK-5 ordered mesoporous carbon” 2015
27. Akshay Bansal on “Classical density theory for confined polar fluids” 2015
28. Nisha Masawan on “ Experimental investigation on nanoparticle adsorption mechanism on cellulose surface” 2015
29. Aman Sharma on “ Shale gas : adsorption and desorption behavior using molecular simulation” 2014
30. Pooja Sahu on “ Process development for grafting of macrocyclic crown ether on a suitable solid matrix for chromatographic separation of metal ion/isotopes” 2013
31. Utsav Kumar on “Multi-scale simulation of Li-ion battery” 2013
32. Haritha B on “Aqueous solution: adsorption behaviour surfactant/ligand in the presence of heavy metal ions: experiments and simulations” 2013
33. Parul Katiyar on “ Understanding mechanical properties of hollow graphite nanofibers and polyethylene composite: experiments and molecular simulation” 2013
34. Atanu Metya on “ Thermodynamics and transport properties of liquid alkali metals in bulk and near surfaces” 2011
35. Rakesh Kanobodia on “ Structural and transport properties of imidazolium based ionic liquids as electrolytes in li-ion batteries” 2011
36. M. V. P. Srinivas on “ Vapor-liquid phase transition of associating fluids under slit-pore confinement” 2010
37. Ravi C. Dutta on “ Wetting properties of water on smooth and textured surfaces: A molecular dynamics study” 2010
38. Abhiram Hens on “Vapor-liquid phase transition of sodium and 2D polymeric fluids” 2010
39. D. J. Naresh on “ Virial equations of states of simple associating and colloidal fluids: A Monte Carlo Study” 2009
40. Subimal Jana on “ Phase behaviour of square-well fluids in slit pores” 2008
41. A. Naresh on “ Vapor-liquid phase coexistence properties of variable square well fluids and on site associate fluids in repulsive porous media” 2008
42. Rohan Awasti on “ Simulation of Direct Methanol Fuel Cell (DMFC)” 2008
43. Ashish Bhateja on “ Axial segregation in horizontally vibrated granular material: A numerical study” 2008

(C) POST-DOCTORAL RESEARCHER

1. Dr. Satyapal Singh (2009-2010)
2. Dr. Rajat Srivastava (2009-2011)
3. Dr. Minakshi Sultania (2010-2011)
4. Dr. Surendra Jain (2012)
5. Dr. Nihar Ranjan Biswal (2015-2017)
6. Dr. Ravi Kant (2014-2015)
7. Dr. Sarabani Ghosh (2016-2017) (NPDF)

8. Dr. Anuj Kumar (2016)
9. Dr. Arun K. Singh (2016-2018) (NPDF)
10. Dr. Preeti Srivastava (2017-2018)
11. Dr. Praveen Sappadi (2017-2019) (NPDF)
12. Dr. Shruti Misra (2017-2020) (Women Young Scientist)
13. Dr. Showkat Mir (2018-2020)
14. Dr. Vivek Yadav (2018- 2019)
15. Dr. Debdip Bhandari (2018-2019)
16. Dr. Reema Biswas (2018- 2019)
17. Dr. Jyoti Sahu (2019-2020)
18. Dr. Debabatra Pramanik (2019-)
19. Dr. N. Sadanandam (2019-20)
20. Dr. Amit Kumawat (2020-2021)
21. Dr. Sujit Das (2020)
22. Dr. Arpita Srivastava (2020-2021)
23. Dr. Vanshree Parey (2021-2022)
24. Dr. Moses Abraram (2020- 2023, NPDF)
25. Dr. A. Nagraj (2021-2023) (NPDF)
26. Dr. Sanchari Bhattarcharya (2021)
27. Dr. M. Jyothirmai (2021-2023)
28. Dr. M. Aamir Khan (2021-2022)
29. Dr. Malay Biswal (2022-2025)
30. Dr. Mayank Gupta (2022)
31. Dr. Bushnagar Adivaiah (2022-2023)
32. Dr. Tamaghna Chakraboti (2023-2025)
33. Dr. Satyabrata Subhodi (2023)
34. Dr. Sangeeta Mahala (2022)
35. Dr. Aswathi Mohan (2023-2024)
36. Dr. M. Jyothirmai (2024-2026) (NPDF)
37. Dr. Sudipta Roy (2024- 2026)
38. Dr. Shirish Updadhya (2024-) (IPDF)
39. Dr. Mona Vishwakarma (2025-2026)
40. Dr. Ardhra S Shyendran (2025-2026)
41. Dr. Raj Akshat (2026-)
42. Dr. Rahul Sahu (2026-)

(D) PROJECT ASSOCIATE RESEARCHER: 32

SPONSORED PROJECTS (Rs ~68 cr)

(A) GOVERNMENT SPONSORED PROJECTS (Rs. 533 M)

1. Force-field development of high-energy materials, DRDO, 2025-2028, Rs 35.84M
2. COE in Speciality Chemical, DCPC, 2025-2030, Rs. 50 M

3. Nature-inspired Insilico design of anti-freeze nanoparticles, SERB, 2024-2027, Rs. 6.6 M
4. R&D of low GWP chemicals, MOEFC, Rs. 5 M
5. CREATE: Centre for rechargeable energy storage system for augmenting transportation and electrification, SERB, 2022-2027 Rs, 84 M
6. DST-BioEnergy and H2 Map, DST, 2022-2025, Rs. 11.4 M.
7. Soil health monitoring for agricultural applications, UP-GOVT, 2021-2022, Rs 5.7 M
8. Development of electrochemical biosensors for detection of emerging pollutants in water, DST, 2020-2023, Rs. 6.992 M
9. Structural evaluation of building blocks of ice in different geometry/conditions and its impact on nucleation behaviour, SERB, 2020-2023, Rs. 3.85 million
10. Development of a hybrid approach for high-throughput screening of material, SERB, 2020-2023, Rs. 0.66 million
11. Understanding the self-assembly of amphiphilic molecules in supercooled solvents using molecular simulations, SERB, 2020-2023, Rs. 6.46 million
12. In silico screening for repurposing known drugs for SARS-COV-2 using AI and molecular simulations, SERB, 2020-2021, Rs. 1.669 million
13. One dimensional model for the study of oxidation modeling of PCS fiber on a stationary cylindric roll, DMSRDE, 2019-2020, Rs. 1.07 million
14. Modeling validation and application of ligand coated soft materials for adsorptive separation of GD^{3+} and UO_2^{2+} ions, DAE-BRNS, 2016-2019, Rs. 4.19 million.
15. Nucleation of nanostructured surface, DST-RFBR, 2017-2019, Rs. 1.5 million.
16. Boron nitride based adsorbent for removal of arsenic from aqueous streams, DST, 2016-2019, Rs 4.26 million.
17. Wetting behavior of fluids in presence of large particles on surfaces, DST-SERB 2015-2018, Rs 5.93 million.
18. Advanced Computation and Research, MHRD, 2013-2018, Rs 57 million.
19. Adsorption and desorption behavior of nanoparticle on a polymeric surface, CSIR, 2015-2018, Rs. 1.567 million.
20. Center of Material Modeling, Mechanics and Applications, MHRD, 2014-2019, Rs 68.9 million.
21. Aligned carbon nanotubes as porous materials for selective carbon dioxide adsorption and desorption: effect of pressure and charges, MOES, 2014-2017, Rs. 4.105 million.
22. Molecular simulation study of the wetting behavior of polymer grafted silica surfaces, DST Indo-Portuguese, 2014-2017, Rs. 0.46 million.
23. Segregation of vibrated granular materials, DST 2011-2014, Rs, 3.38 million.
24. Polymer-nanofiber separator for batteries, DST, 2011-2014, Rs 4.14 million.
25. Wetting behaviour of aqueous organic fluids on functional surfaces, UP-CST, 2010-2013, Rs 0.6 million.
26. Molecular simulation of wetting transitions of functional surfaces, CSIR, 2009-2012, Rs 1.2 million.
27. Structural and dynamical properties of organic and aqueous fluids at nanoscale, DST, 2010-2013, Rs 3.35 million.
28. Setting up of a supercomputing facility at IIT Kanpur, DST, 2010-2013, Rs 99.6 million.

29. Improving the wettability of liquid Sodium on Metal/Alloys, DAE-IGCAR, 2009-2011, Rs 1.586 million.
30. Monte Carlo Simulation Study of Metal-Ion Solvent Systems, DAE-BRNS 2009-2012, Rs 3.625 million.
31. Mesosstructured Functional Thin Films and Interfaces of Soft Materials, IRPHA, DST, 2007-2011, Rs 49.5 million.
32. Segregation in Heterogeneous Media, IIT Kanpur, 2007-2010, Rs 0.5 million.
33. Molecular simulation of associating fluids and their mixtures. DAE-BRNS, 2006-2009, 1 million.
34. Phase equilibria and interfacial properties of fluid and their mixture in nanoporous materials, DST, New Delhi, 2006-2009, 1.881 million.
35. Structure, dynamics and phase behavior of complex fluids via Molecular Simulation, IIT Kanpur, 2006-2007, 0.9 million.

(B) INDUSTRY/CSR SPONSORED PROJECTS (Rs. 147 M)

1. COE for Speciality Chemicals, 2025, Rs 25M
2. AI for Engineering Science Lab, 2025, Rs. 30 M
3. Role Of Multifunctional Actives On Modulating Water Activity And Microstructure Of Mixed Surfactant Systems : Effect Of Formulation Preservation, 2025-2027, Unilever, Rs.5.3 M
4. Development of Soil Sensor for Micronutrients, 2025, Kotak CSR, Rs. 3.0 M
5. Understanding the Relation of Water Activity and Microstructure of Mixed Surfactant Systems on Preservative Efficacy, 2024-2025, Unilever, Rs 4.8 M
6. Development of Framework to Screen Lubricants, Khanna and Khanna, 2023-2024, Rs 1.5 M
7. Effect of water activity and micro surfactant of mixed surfactant system on preservative efficacy, Unilever, 2023-2024, Rs. 3 M.
8. Development of Indigenous integrated carbon capture and conversion (ICCC) technology, BPCL, 2023-2025 Rs. 9.996 M
9. Extraction of titanium salts, Nisarg Ispat Pvt. Ltd, 2023, Rs. 3.3 M
10. Technology for health care, SLPL, 2023-2025, Rs. 5.0 M
11. Development of Lab Scale Process for Separation of TIO₂, Nisarg Ispat Pvt. Ltd, 2022, Rs. 2.6 M
12. Pilot Scale Demonstration of liquid phase sulfonation of aliphatic, alkyl aryl and aromatic alkylates, Technithon Pvt. Ltd., 2022-2024, Rs. 11.3 M
13. Predicting Ion Conductivity and deducing structure-property relationships for hydrated anion exchange membranes using molecular dynamics simulations, Shell, 2022-2025, Rs 9.3 M
14. Project Activities of scientific research in developing portable oral cancer detection device, 2021-2024, LIC HFL, Rs. 10.6 M
15. Development of an interactive cloud based diagnostic platform for oral cancer, Postescap India, 2021-2023, Rs. 3.8 M
16. Impact of humidity and temperature on the structural changes of salt hydrates, Unilever Ltd. 2021-2022, Rs. 1.79 M

17. Phase Diagram of Salt Hydrate in Presence of Surfactant, Unilever Ltd. 2019-2020, Rs. 1.79 M
18. Development of Soil Testing Tool, RTPL, 2019-2020, Rs 1.0 M
19. Predicting the Release of Drugs from Multi-component Supramolecular Membranes, Akimara Biomedicine Pvt. Ltd, 2019-2020, Rs. 1.03 M
20. Martinizing Anti-Cancer Drugs and Optimizing Multi-Component Supramolecular Formulations, Invictus Oncology, 2018-2019, Rs. 1.03 M
21. Research and Development for Chemical Technology, SLPL, 2017-2022, Rs. 7.5 M
22. Understanding adsorption-desorption mechanism of nanoparticles on surfaces, Unilever, 2013-2014, Rs 1.55 M.
23. Development of extra light and strong anti-weathering nets, Ingen, 2011-12, Rs 0.73 M
24. Electronic, Optical, Structural and Dynamical Properties of ZnS-PMMA Nanocomposite, Samsung R&D, 2011-2012, Rs 2.50 M
25. Understanding the nanoscale properties related to diffusion, surface stress and modulus of lithium ion cell materials using atomistic simulations, General Motors, 2011-2012, Rs 3.1 M

PROFESSIONAL SERVICES

(A) PROFESSIONAL ACTIVITIES [1] [SEP]

1. Regional Coordinator of INAE-Infosys Center for Engineering Education Excellence 2025-
2. Coordinator of INSA Leadership Development Programme in Science & Technology (LEADS) 2024
3. Coordinator of DST-SATHI meeting, November 4, 2023.
4. Co-Coordinator of INSA Leadership Development Programme in Science & Technology (LEADS) 2023
5. Member of Task force for CCUS (Niti Ayog & Ministry of Steel) 2023
6. Member of DST Task Force for further enhancing infrastructure - 2023
7. Member of the selection committees in IITs, BITS Mesra, NITs and AKTU.
8. Member of PAC for MATRICS -2020
9. Member of National Committee for DST NPDF, ECR, and Chemical and Environmental Engineering PAC (2018-2020)
10. Organising member of LEAP, IIT Kanpur, November 19-30, 2018
11. Session Chair, Computational Method, COMFLU, Roorkee, December 9, 2018
12. Session chair, A discussion meeting on “Recent Advances in Molecular Simulations”, IISc Bangalore, 8-11 February 2018.
13. Organising member, Computational Molecular Engineering, HiPC 2016, Hyderabad, 19 December 2016.
14. Associate Editor, Chemical Engineering Communication, Taylor and Francis, 2016-
15. Session Chair and Organising member of Indo-German Frontiers of Engineering 2015, Agra, February 19-22 2015.
16. Session Chair, European Society of Applied Thermodynamics (ESAT) 2014
17. Session Chair, Current Trends in Theoretical Chemistry, 2013
18. Member of Editorial Board of The Scientific World Journal, 2013-2017
19. Session Chair (Presiding), Foundation of Molecular Modeling and Simulation, Portland, July 22-26, 2012
20. Session Chair, Nanotechnology, National Conference on Frontiers in Chemical Engineering, 2007, IIT G
21. Organizing member of INDO-US conference on Fabrionics: Advanced Fabrication, IIT Kanpur, 2010, IIT K
22. Member of high level committee HPC facilities of ministry of earth sciences-2012
23. **Reviewer** for Phys. Rev. Letts.; Langmuir; J. Chem. Phys.; Scientific Reports; J. Phys. Chem. A, B, C; J. Am. Chem. Soc.; Macromolecules; Theo. Chem. Acc.; Phys. A; Chem. Phys.; Chem. Phys. Letts.; Fluid Phase Equil.; Mol. Phys.; Mol. Sim.; Appl. Phys. Lett.; RSC Adv.; Nanoscale; J. Phy. Chem. Letters; Coll. Czech. Chem. Comm; Int. J. of Eng. Sci. Tech. (IJEST), Appl. Surf. Sci.; Chem. Eng. Sci.; Soft Matter; Mat Sci Eng C; AIChE; Ind. Eng. Chem. Res.; J. Colloid & Interface Sci.; Indo-US Science & Technology Forum; SERB, DST.
24. **External Examiner** for M.Sc. and Ph.D. theses [1]
[SEP] of Queensland University, Indian Institute of Science, Bangalore, IIT Madras, IIT Guwahati, IIT Kharagpur, IIT Roorkee, IIT Bombay and IISERs.

(B) CONTINUING EDUCATION ACTIVITIES

1. Coordinator, Fundamentals of Molecular Simulations (FunMolSim 2020) Feb 17-21, IIT Kanpur, 2020
2. Coordinator, Molecular simulations of complex fluids and interfaces, Feb 21-23, IIT Kanpur, 2020
3. Coordinator, IITK-AKTU, FDP program 2019 (conducted over 12 courses covering 400 colleges of UP, and 600 faculty).
4. Coordinator, Fundamentals of Molecular Simulations (FunMolSim) 2019, March 5-9, 2019
5. Convener SERC School-cum-Symposium on molecular simulation November 27-30, 2012
6. Delivered a lecture in Molecular Modeling workshop at UICT, Mumbai, Jan, 2012.
7. Delivered a lecture in ICTS School on "Understanding Molecular Simulations: Theory and Applications" UMS(2010) held at IIT Kanpur during November 4-13, 2010.
8. Delivered a lecture in SERC School on Molecular Simulations for Chemical engineers, IISc Bangalore, May, 2009

(C) ADMINISTRATIVE SERVICES (IIT KANPUR)

- | | |
|---|-------------------------|
| 1. Professor In charge Infrastructure & Planning, IITK | 2025- 2026 |
| 2. Chairman, Construction of GSMST(Medical School), IIT K | 2024- 2026 |
| 3. Head, Department of Chemical Engineering | 2022-2024 |
| 4. Director, IITKDF (section 8 company) | 2020-2022 |
| 5. Secretary, Alumni Association IIT Kanpur | 2019-2021 |
| 6. Dean of Resource and Alumni, IIT Kanpur | 2019-2022 |
| 7. Head, CDTE/QIP | 2018-2019 |
| 8. Nodal Coordinator, National Supercomputing Mission | 2017-2020 |
| 9. HPC Convener | 2016-2020 |
| 10. Associate Dean, UG program | 2016-2018 |
| 11. Student Award committee member | 2013-2014 |
| 12. S-SAC member | 2011-2012 |
| 13. Treasurer, Alumni Association IIT Kanpur | 2010-2012 |
| 14. DPGC convener | 2010-2012 |
| 15. DPGC committee member | 2008-2010;
2013-2014 |
| 16. Warden-in-charge, Hall II | 12/2008-05/2009 |
| 17. Chemineer Faculty-in-charge | 04/2006-04/2009 |
| 18. Maintenance and Mess Warden, Hall II | 12/2007-12/2008 |
| 19. CCCC representative | 2008 |
| 20. Faculty Counselor | 2006-2008 |

(D) Institutional Building Activities (IIT KANPUR)

1. Led the initiative to raise funds to create 'Chemical Engineering Annex' building - 2026
2. Initiated major projects of worth 300 cr during 1 year of PIC of infrastructural & planning of IIT Kanpur
3. Establishment of supercomputing facility (Raised over 150 cr from internal and external sources)
 - a. Founding member and coordinator of the first HPC facility of IITK, HPC 2010 and later HPC 2013.
 - b. Founding member of NSM facility, Param Sanganak, 2021
4. Founder Director of IITK Development Foundation 2020-22
 - Raised 350 crore in 3 years
 - Designed and created many background platforms, Alumni database management system and Donation Management System, to accelerate the fundraising and enhancing the quality of interaction with alums.
 - Created process, restructure offices, and automated all the key processes for smooth operation
 - Developed AlmaWorld to bring alumni closer to the institute and to have a reunion platform for ease of operation.
 - Raised funds to create Gangawal School of Medical Science and Technology
 - Raised funds to create centres ranging from Rozi Siksha Kendra to Center for Neurodegenerative diseases.
5. Founding member of Sustainable Energy Engineering 2021
 - a. Created new department and two centres primarily focusing on energy engineering along with other members.
6. Establishing new Undergraduate Lab of chemical engineering department and Graduate Student Lounge (first in IITK) 2022-23