

# Curriculum Vitae

**Name:** Jayant Kumar Singh

**Date of Birth:** February 03, 1975 ( Buxar, Bihar)

**Designation:** Chair Professor (HAG)

**Address** Department of Chemical Engineering

Institute of Technology Kanpur

Kanpur, UP-208016

Tel: +91-512-2596141, Fax: +91-512-2590104

Email: [jayantks@iitk.ac.in](mailto:jayantks@iitk.ac.in)

Web: <https://cnislab.com>

## 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

## Awards and Honors

- 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 (INAE) 2022
- Herdillia Award, IChE 2021
- Elected Fellow, National Academy of Science, India (NASI) 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

### Field of Specialization

- Gas separation & Storage (CO<sub>2</sub> capture)
- Drug, material and speciality chemical discovery
- Statistical mechanics, Thermodynamics, and molecular simulations
- Machine learning & AI based disruptive technologies

### Experience

HAG Professor	August 2022-	Department of Chemical Engineering, IIT Kanpur
Head	January 2022-	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
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. 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 a company.
2. 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)
3. 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)
4. Singh JK, Prince P, Ahmad A, Khan MA and Khemani Y, *Portable Smart Device for Determination of Soil Nutrients* (applied, 2020, granted 2024; IPA Application No : 202011056711 | PCT application number: PCT/IB2021/062229)
  - a. Technology is transferred and licensed (for Indian Market) to **AgroNxt Pvt. Ltd.**
5. Singh JK, Singh P, Khan A, Rupaliya A and Kemani, Y, *Muhn Parikshak: Oral Cancer Testing Device*. (applied, 2024)
6. Singh JK, Khan A and Gupta A, *Karn Parikshak: Portable Otoscope for detection of various ear diseases*. (applied, 2024)

### (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 CO<sub>2</sub> 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), 1<sup>st</sup> Edition 2009 (ISBN: 978-1441915429).

**(E) IN REFEREED JOURNALS (186, h-index=39)**

1. Bhendele M, Sharma R and Singh JK, Cosolvent Induced Phase Transitions in ABA Block Copolymers: A Molecular Dynamics Study, *submitted*.
2. Krishnan SM, Sharma R, and Singh JK, *CoRE MOF screening for Propane adsorption refrigeration* submitted
3. Bhendele M, Singh JK, Zaccone A, *Enhanced molecular diffusivity in sheared supercooled liquids*, submitted

4. Tamagna, Riya, Anand and Singh, Unravelling the effect of molecular interactions on macroscale properties in Sustainion AEM under hydrated conditions using MD simulations, *submitted*.
5. Abraham B , Sinha P and Singh JK, Machine Learning for Hydrogen Evolution Reaction: Physical Insights from Classical Data, *submitted*.
6. Aqib M, Daoo V and Singh JK, Efficient Xylene Isomer Separation: Accelerated Screening with Active Learning and Molecular Simulation, *Energy & Fuels submitted*
7. Biswal M, Roy S and Singh JK, In Silico Engineering of Stable siRNA Lipid Nanoparticles: Exploring the Impact of Ionizable Lipid Concentrations for Enhanced Formulation Stability, *Submitted*.
8. Shrivastava D et al., Large area film of cleavable and transferable semi-conducting two dimensional Imine-COF, *submitted*
9. Abraham B, Sinha P and Singh JK, 2D MXene with Functionalisation for Hydrogen Evolution Reaction, *submitted*
10. Jyothirmai MV, et al, Machine Learning Driven High-Throughput Screening of Transition Metal Atom Intercalated g-C<sub>3</sub>N<sub>4</sub>/MX<sub>2</sub> (M = Mo, W; X = S, Se, Te) Heterostructures for Hydrogen Evolution Reaction, *ACS Applied and Interfaces*, accepted, 2024
11. 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*, accepted, 2024.
12. Athawale A, Abraham B, Jyothimai MV and Singh JK, MXene-Based Single Atom Catalysts for Electrochemical Reduction of CO<sub>2</sub> to Hydrocarbon Fuels, *Journal of Physical Chemistry C*, 127,24542-24551, 2023.
13. Bhendele M, Indra A, Singh JK, Does freezing induces self-assembly of polymers? A molecular dynamics study, *Soft Matter*, 19,7570-7579, 2023.
14. Parey V, Abraham B, and Singh JK, Surface Hydroxylation Mechanism of Zr<sub>2</sub>X(OH)<sub>2</sub> (X = C, N, or B) MXenes: A Promising Catalyst for CO<sub>2</sub> Conversion into Formic Acid. *Materials Chemistry and Physics*, 310,128444, 2023.
15. Gupta M, Daoo V and Singh JK, Amine decorated MOF for direct capture for CO<sub>2</sub> from ambient air, *Dalton Transaction*, 52, 11621-11630, 2023.

16. 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.
17. Srirangam S, Bhendle M and Singh JK, Is Universal Shear Behavior of supercooled water retained at higher pressures, accepted *Physical Chemistry Chemical Physics*, 25, 21528-21537, 2023.
18. Abraham B, et al, Integrating Machine Learning and Molecular Simulation for material design and discovery, *Transaction INAE*, 8,325-340 2023.
19. 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*, 127, 17039-17050, 2023.
20. 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*, 384,122261, 2023.
21. Abraham M et al Machine learning-driven discovery of key descriptors for CO<sub>2</sub> activation over two-dimensional transition metal carbides and nitrides, *ACS Applied Materials and Interfaces*, 15, 30117-30126, 2023.
22. Jyothimai D, Roshni M. V. Abraham M and Singh JK, Accelerating the Discovery of g-C<sub>3</sub>N<sub>4</sub> Supported Single Atoms Catalysts for Evolution Reaction: A Combined DFT and Machine Learning Strategy, *ACS Applied Energy Materials*, 10, 5598-5606, 2023.
23. 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.
24. 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.
25. Halder P and Singh JK, Screening of Hypothetical Metal Organic Frameworks for Xylene Isomers and Ethylbenzene Separation, *Energy & Fuels*, 37, 2230-2236, 2023.
26. 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.

27. Mir SH, Yadav VK and Singh JK, Efficient CO<sub>2</sub> capture and activation on novel two-dimension metal borides, *ACS Applied Material Interfaces*, 14, 29703-29710, 2022.
28. 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.
29. 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.
30. 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.
31. 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*, *Journal of Computational Chemistry*, 43, 1237-1250, 2022.
32. 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.
33. Parey V, Abraham BM, Jyothirmai and Singh JK, Mechanistic Insights for Electrochemical Reduction of CO<sub>2</sub> into Hydrocarbon Fuels over O-Terminated MXenes, *Catalysis Science and Technology*, 12, 2223-2231, 2022.
34. 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.
35. 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.
36. 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.
37. K Suraj, Goswami A, Singh JK, Salt-Water System under Diamond Confinement, *Journal of Physical Chemistry C*, 125, 22283-22294, 2021.



38. Tewari S, Abraham BM, Singh JK, Insight into the mechanism of nanoparticle induced suppression of interfacial tension, *Journal of Molecular Liquid*, 339, 117177, 2021.
39. 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.
40. Goswami A, Dalal IS, Singh JK, Universal Nucleation Behavior of Sheared Systems, *Physical Review Letters*, 126, 195702, 2021
41. Parey V, Abraham BM, Mir S and Singh JK High-throughput screening of atomic defects in MXenes for CO<sub>2</sub> capture, activation and dissociation, *ACS Applied Materials & Interfaces*, 13, 35585-35594, 2021.
42. 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.
43. Goswami A and Singh JK, A Hybrid Topological and Shape-Matching Approach for Structure Analysis, *Journal of Chemical Physics*, 154, 154502, 2021.
44. 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.
45. 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.
46. Goswami A, Dalal IS and Singh JK, Seeding Method for Ice Nucleation under Shear. *Journal of Chemical Physics*, 153, 094502, 2020
47. 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
48. 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
49. Maurya M and Singh JK, Selective separation of CO<sub>2</sub> from flue gas using carbon and boron nitride nanotubes as a membrane, *Energy & Fuels*, 34, 7223-7231, 2020
50. 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

51. Mir SH, Yadav VK and Singh JK, Electronic properties and superior CO<sub>2</sub> capture selectivity of metal nitride (XN) and phosphide (XP) (X = Al, Ga and In) sheets, *Applied Surface Science*, 527,146445, 2020.
52. 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
53. 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*
54. 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.
55. 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**).
56. 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.
57. 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.
58. Saha P, Yadav V, Gurunarayanan 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.
59. 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.
60. Sappidi P and Singh JK, Molecular dynamics study on the adsorption of UO<sub>2</sub><sup>2+</sup> 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**).
61. 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.

62. 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.
63. Saha P, Yadav, Gurunarayanan, 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, 18488-184494, 2019.
64. 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**).
65. 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.
66. 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.
67. 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.
68. Sappidi P, Boda A, Ali SK and Singh JK, Adsorption of gadolinium (Gd<sup>3+</sup>) 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.
69. 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.
70. 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.
71. 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.
72. 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.

73. 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.
74. 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.
75. Ghosh S and Singh JK, Hydrogen adsorption in pyridine bridged porphyrin-covalent organic framework, *International Journal of Hydrogen Energy*, 44, 1782-1796, 2019.
76. Metya AK and Singh JK, Ice adhesion mechanism on lubricant-impregnated surfaces using molecular dynamics simulations, *Molecular Simulation*, 45, 394-402, 2019.
77. Sappidi P, Mir SH and Singh JK, Effect of polystyrene length for the extraction of Gd<sup>3+</sup> and UO<sub>2</sub><sup>2+</sup> ions using dicyclohexano crown ether (DCH18C6) with octanol and nitrobenzene: A molecular dynamics study, *Journal of Molecular Liquids*, 271, 166-174, 2018.
78. Maurya M and Singh JK, Treatment of flue gas using graphene sponge: A simulation study, *Journal of Physical Chemistry C*, 122, 14654-14664, 2018.
79. Metya AK and Singh JK, Ice nucleation on a graphite surface in the presence of nanoparticles, *Journal of Physical Chemistry C*, 122, 19056-19066, 2018.
80. Majumdar S, Maurya M and Singh JK, Adsorptive separation of CO<sub>2</sub> from multicomponent mixtures of flue gas in carbon nanotube arrays: A grand canonical Monte Carlo study, *Energy Fuels*, 32, 6090-6097, 2018.
81. Metya A and Singh JK, Nucleation of aqueous salt solutions on solid surfaces, *Journal of Physical Chemistry C*, 122, 8277-8287, 2018.
82. Katiyar P and Singh JK, The effect of ionization of silica nanoparticles on the adsorption of nonionic surfactants at oil-water interface: An atomistic molecular dynamic study, *Molecular Physics*, 116, 2022-2031, 2018.
83. Xuan P, Jain S, Singh JK, Liu A and Jin Q, Formation patterns of water clusters in CMK-3 and CMK-5 Mesoporous Carbons: A computational recognition study, *Physical Chemistry Chemical Physics*, 20, 17093-17104, 2018.
84. Namsani S and Singh JK, Enhancement of thermal energy transport across the gold-graphene interface using nanoscale defects: A molecular dynamics study, *Journal of Physical Chemistry C*, 122, 2113-2121, 2018.

85. Shevkunov SV and Singh JK, Bicanonical ensemble Monte Carlo simulation of water condensation in the field of crystal lattice defects, *Journal of Molecular Liquids*, 264, 150-164, 2018.
86. Sappidi PK, Namsani, Ali SM and Singh JK, Extraction of Gd<sup>3+</sup> and UO<sub>2</sub><sup>2+</sup> ions using polystyrene grafted dibenzo crown ether (DB18C6) with octanol and nitrobenzene: A molecular dynamics study, *Journal of Physical Chemistry B*, 122, 1334-1344, 2018.
87. Kommu A and Singh JK, Removal of Pb(II) ion using PAMAM dendrimer grafted graphene and graphene oxide surfaces: A molecular dynamics study, *Journal of Physical Chemistry A*, 121, 9320-9329, 2017.
88. Namsani S, Auluck S and Singh JK, Thermal conductivity of thermoelectric material  $\beta$ -Cu<sub>2</sub>Se: Implications on phonon thermal transport, *Applied Physics Letters*, 111, 163903 2017.
89. Singh AK, Kumar K and Singh JK, Simple and green fabrication of recyclable magnetic highly hydrophobic sorbents derived from waste orange peels for removal of oil and organic solvents from water surface, *Journal of Environment Chemical Engineering*, 5, 5250-5259, 2017.
90. Sinha N and Singh JK, Effect of nanoparticles on the vapour-liquid surface tension of water: A molecular dynamics study, *Journal of Molecular Liquids*, 246, 244-250, 2017.
91. Katiyar P and Singh JK, A coarse-grain molecular dynamics study of oil-water interfaces in the presence of silica nanoparticles and nonionic surfactants, *Journal of Chemical Physics*, 146, 204702, 2017.
92. Singh AK and Singh JK, Fabrication of durable superhydrophobic coating on cotton fabrics with photocatalytic activity by fluorine-free chemical modification for oil-water separation, *New Journal of Chemistry*, 41, 4618-4628, 2017.
93. Singh AK and Singh JK, Simple and green fabrication of super-repellent surfaces on cotton fabric with liquids of varying surface tension, *Applied Surface Science*, 416, 639-648, 2017.
94. Peng X, Jain S and Singh JK, Separation of N<sub>2</sub>/CH<sub>4</sub>/CO<sub>2</sub>/SO<sub>2</sub> gases in disordered carbons obtained using hybrid reverse Monte Carlo simulation, *Journal of Physical Chemistry C*, 121, 13457-13473, 2017.
95. Namsani S, Auluck S, Bhaskar G and Singh JK, An Interaction potential to study the thermal structure evolution of a thermoelectric material:  $\beta$ -Cu<sub>2</sub>Se, *Journal of Computational Chemistry*, 38, 2161-2170, 2017.

96. Bhateja A, Sharma A and Singh JK, Segregation physics of a macro-scale granular ratchet, *Physical Review Fluids*, 2, 05301 (R), 2017.
97. Srivastava R, Kommu A, Sinha N, and Singh JK, Adsorption of Arsenic ions on Boron Nitride and Graphene surfaces, *Molecular Simulation*, 43, 985-996, 2017.
98. Kommu A and Singh JK, Separation of ethanol and water using graphene and hexagonal boron nitride slit pores: A molecular dynamics study, *Journal of Physical Chemistry C*, 121, 7867-7880, 2017.
99. Bhandary D, Velachi V, Bhandary D, Dias Soeiro Cordeiro MN and Singh JK, Janus gold nanoparticles from nano droplets of alkyl thiolates: A molecular dynamics study, *Langmuir*, 33, 3056-3067, 2017.
100. Maurya M and Singh JK, Capture of SO<sub>2</sub> using functionalized bilayer graphene nanoribbons, *Journal of Chemical Physics*, 146, 044704, 2017.
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## **(F) INVITED TALKS**

1. Singh JK, *Machine learning and molecular simulation integrated approach for material design and discovery*, BASF India, Mumbai, Feb 28, 2024.
2. Singh JK, Supercooled water in the presence of nanostructured surface and under shear flow, ICMS, Taiwan, October 5-9, 2023
3. Singh JK, Decoding the Chemistry of 2D MXenes for CO<sub>2</sub> Capture and Conversion Through Machine Learning, CEES, IIT Mandi, September, 26, 2023
4. Singh JK, Insight into ice formation at extreme confinement and under shear flow, Department of Physical Chemistry, University of Barcelona, May 26, 2022.
5. Singh JK, Nuclear under shear flow, INAE annual convention, December 14-16, 2022.
6. Singh JK, New Insight into the ice formation: extreme confinement & under shear flow, IIT Bombay, January 2022.
7. Singh JK, New Insight into the ice formation: extreme confinement & under shear flow, Theoretical Chemistry Symposium, December 11-14, 2021.
8. 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.

9. Singh JK, Fundamentals of Wetting Transitions, Hindustan Unilever Ltd, April 15, 2020
10. 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
11. Singh JK, Unraveling nanoconfined world using molecular simulations, December 6, COMFLU-2019
12. Singh JK, What nanoparticles can do to bulk and interfacial properties? University of Crete, Greece, May 29, 2019
13. Singh JK, Insights into material behavior via molecular simulations, *Invictus Oncology Pvt. Ltd.* Delhi, October 24, 2018
14. Singh JK, *Fourth industrial revolution*, LEAP, IIT Kanpur, November 20, 2018
15. Singh JK, *Ice nucleation in presence of foreign substances*, Department of Chemistry, TU Darmstadt, June 12, 2018
16. Singh JK, *Ice nucleation in presence of foreign substances*, Department of Chemical and Biological Engineering, NUS, May 21, 2018
17. Singh JK, *Multi-scale simulations of energy materials: some case studies*, Shell India, R&D, April 12, 2018
18. Singh JK, *Phonon thermal transport in  $\beta$ -Cu<sub>2</sub>Se using an ab initio derived force-field*, Discussion Meeting on Recent Advances in Molecular Simulations, IISc Bangalore, February 08-11, 2018
19. Singh JK, *Changing world of chemical engineering*, Ujjain Engineering College, 24 March, 2018
20. Singh JK, *Changing world of chemical engineering*, Madan Mohan Malaviya University of Technology, Gorakhpur, February 11, 2018
21. Singh JK, *Molecular insight into nucleation behavior of supercooled water on surfaces*. IMS, Japan, May 18, 2017
22. Singh JK, *What we can learn about nucleation of supercooled water on surfaces using molecular simulation ?* Okayama University, May 15, 2017
23. Singh JK, *Nanoparticles aggregation and dispersion behaviour, and its effect on thermophysical properties*, Jilin University, October 27, 2016
24. Singh JK, *Molecular insight into fluid behavior near substrate*, Univ Porto, Porto, June 28, 2016

25. Singh JK, *Understanding ice nucleation on nanostructured surfaces*, TU Darmstadt, June 19, 2016
26. Singh JK, *Understanding water behavior on soft/hard surfaces using molecular simulations*, TU Kaiserslautern, May 17, 2016
27. Singh JK, *Molecular insight into fluid behavior near substrate*, IISc Bangalore, April 7, 2016
28. 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
29. Singh JK, *Understanding the formation of Janus particles from nano droplets of alkyl thiols*, Tutzing, Germany, October 21, 2015
30. Singh JK, *Understanding the behavior of supercooled liquid in presence of surfaces using molecular simulations*, Institute of Thermodynamics, Univ. Stuttgart, Germany, July 07, 2015
31. Singh JK, *Understanding water(ice)-surface behavior*, Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung (IFAM), Bremen, Germany, June 25, 2015
32. Singh JK, *Coarse-grained molecular simulations of nanoparticles and nanocomposites*, BARC, January 16, 2015
33. Singh JK, *Oscillatory behavior of melting behavior of nanoconfined fluids*, TCS 2014, NCL Pune, December 18, 2014
34. Singh JK, *Solid-liquid transition of nanoconfined fluids*, TU Kaiserslautern, Germany, July 15, 2014
35. Singh JK, *Phase transitions of nanoconfined fluids*, SN Bose Institute Kolkatta, April 11, 2014
36. 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
37. Singh JK, *Understanding phase transition at nanoscale: role of external field*, Univ at Porto, 04 December, 2012
38. Singh JK, *Cross over behavior of confined fluids: 3D to 2D*, TU Darmstadt, Germany, July 19, 2012
39. Singh JK, *Phase transitions at nanoscale: role of confinement*, TU Darmstadt, Germany, July 19, 2012

40. Singh JK, *Unveiling thermodynamics at nanoscale*. Planetary Lecture, IChE Annual Meeting, Annamalai University, December, 2010.
41. Singh JK, *Fluid near surfaces*, Department of Polymer Engineering, BITS Ranchi, January 29, 2010.
42. Singh JK, *Fluid near surfaces*, Department of chemical and biomolecular engineering, Vanderbilt University, November 23, USA, 2009.
43. Singh JK, *Molecular modeling and simulation of fluids near surfaces*, Modeling and simulation of chemical processes, HBTI Kanpur, February, 2009.
44. Singh JK, *Molecular modeling and simulation: Can it help in the development of micro and nano devices?*, INDO- US Workshop, IIT Kharagpur, 2009.
45. Singh JK, *Molecular simulation of fluids near surfaces*, HPC workshop, IISc Bangalore, November 2008.
46. Singh JK, *Fluids near surfaces*, Department of Mechanical Engineering, IIT Kanpur, September 2008.
47. Singh JK, *Multi-scale simulation of cluster formation and self Assembly*, Indo-US workshop, IIT Kanpur , 2007.
48. Singh JK, *Advanced methods for calculating cluster integrals and interfacial properties*, Department of Chemical Engineering, IIT Delhi, 2004.
49. Singh JK, *Advanced methods for calculating cluster integrals and interfacial properties*, Department of Chemical Engineering, IIT Kanpur, 2004.

## (G) CONFERENCE PRESENTATIONS

50. Indra A, Bhendale M and Singh JK, *Understanding the Role of Polymers on the Nucleating Behavior of Water in Dilute Supercooled Solutions Using Molecular Dynamics Simulations*, AIChE, November 5-9, Orlando, FL, 2023 USA
51. Indra A, Bhendale M and Singh JK, *Understanding the Ice Recrystallisation Inhibition(IRI) activity of Polymer PVA using Molecular Dynamics Simulation*. Complex Fluids Symposium (CompFlu), December 19-21, 2022, Kolkata, India.
52. Bhendale M and Singh JK, *Interdigitated Aggregation of Polymer Surfactant System: A Coarse-Grained Molecular Dynamics Study*. Thermodynamics, September 7-9, 2022, Bath, United Kingdom (Oral & Poster).
53. Bhendale M, Srivasatava A and Singh JK, *Insight into thermodynamics and morphology of different phases of Pluronic L64 from molecular simulations using derived coarse-grained model*. European Symposium on Applied Thermodynamics (ESAT), July 17-19, 2022, Graz, Austria (Oral).



54. Halder P, Prerna and Singh JK, Building unit extraction package for metal-organic framework, ACS Spring 2021, April 5-30, 2021, Online
55. Abram M and Singh JK, *High-Throughput Screening of Atomic Defects in MXenes for CO<sub>2</sub> Capture, Activation, and Dissociation*, MRS Brazil (online) 2021
56. Tiwari S and Singh JK, *Insight into the mechanism of nanoparticle induced suppression of detergency: Theory, Modeling and Simulations*, **ESAT (online), 2020**
57. Pramanik, D and Singh, JK, *Learning reaction coordinate on-the-fly for sampling complex biomolecular systems with SGOOP and metadynamics*, e-Conference on Soft Matter (eCoSoM-2020), Sathyabama Institute of Science and Technology, Chennai, India. July 15-17, 2020,
58. Mir S, Yadav V and Singh JK, *First principle study of two-dimensional materials for environmental applications*, ICMS, November 3-6, 2019, Jeju, South Korea
59. Mishra S and Singh JK, *Simultaneous removal of multiple heavy metal ions from industrial area groundwater by a novel FeS/CFFO/PVDF hybrid nanocomposite membrane*, IGSTC-IGWMWE, February, 18-20, 2019, CSIR-CSMCRI, Bhavnagar, Gujrat, India
60. Mishra S and Singh JK, *Development of novel mixed matrix nanocomposite membrane for simultaneous separation of heavy metals from contaminated water: Application in real water treatment*, 6th IWA-RMTC, December, 10-12, 2018, Maharaja Sayajirao University of Baroda, Gujrat. India
61. Mir SH, Yadav VK and Singh JK, *First principles study of hydrogen evolution reaction on two dimensional boroncarbournitride in waste-water: a comparative study with graphene and hexagonal boron nitride*, TCS 2019, February 13-16 2019, Bits pilani Rajasthan, India
62. Yadav VK and Singh JK, *First Principle Simulation Study of Two-Dimensional Molecular Films for Opto-Electronic Applications*, 16<sup>th</sup> Theoretical Chemistry Symposium, February 13-16, 2019, BITS Pilani, India
63. Maurya M and Singh JK, *Sequestration of SO<sub>2</sub>/CO<sub>2</sub> from flue gas using Graphene sponge - a simulation study*, Carbon Capture and its utilization, December 14-15, 2018, National Chemical Laboratory, Pune, India
64. Maurya M and Singh JK, *Sequestration of SO<sub>2</sub>/CO<sub>2</sub> from flue gas using graphene sponge - a simulation study*, MRS Fall Meeting and Exhibit, Nov 25, 2018, Boston, Massachusetts, USA
65. Metya AK and Singh JK, *Nucleation of aqueous salt solutions on solid surfaces*, Liblice 2018, June17-22, Srni, Czech Republic, 2018

66. Metya AK and Singh JK, *Nucleation of aqueous salt solutions on solid surfaces*, Thermodynamics, September 05-08, Edinburgh, 2017
67. Katiyar P and Singh JK, *A coarse-grain molecular dynamics study of oil–water interfaces in the presence of silica nanoparticles and nonionic surfactants*, September 05-08, Edinburgh, 2017
68. Maurya M and Singh JK, *Sequestration of SO<sub>2</sub>/CO<sub>2</sub> from flue gas using Graphene sponge - a simulation study*, CompFlu, December 18-20, 2017, IIT Madras, Chennai, India.
69. Namasani S and Singh JK, *Tuning the gold-graphene interface thermal conductance by vacancy defects*, ICMS, October 23-26, Shanghai, 2016
70. K Anitha and Singh JK, *Structural and dynamic properties of ethanol-water mixtures in graphene and hexagonal boron nitride slit pores*, AIChE, November 13-18, 2016, San Francisco, CA, USA.
71. Katiyar P and Singh JK, *Understanding adsorption behavior of silica nanoparticles over a cellulose surface in an aqueous medium*, Faraday Discussion, February 6-9, 2016, IIT Mumbai, India
72. K Anitha, Namasani S and Singh JK, *Molecular dynamics simulations of heavy metal ion rejection through functionalized nanopores graphene membrane*, ChEmference2015 IIT Hyderabad, December 5-6, 2015, Hyderabad, India
73. Namasani S and Singh JK, *Tuning the gold-graphene interface thermal conductance by vacancy defects*, National Materials Day, November 11, IIT Kanpur, 2016, India
74. Bhandary D, Benkova Z, Cordeiro MNDS and Singh JK, *Wetting behaviour of grafted thermoresponsive PNIPAAm brushes: A molecular dynamics study*, APMAS2016 1-3 June, 2016, Istanbul, Turkey.
75. Katiyar P and Singh JK, *Understanding adsorption behavior of silica nanoparticles over a cellulose surface in an aqueous medium*, Faraday Discussion, February 6-9, 2016, IIT Mumbai, India.
76. K Anitha, Namasani S and Singh JK, *Molecular dynamics simulations of heavy metal ion rejection through functionalized nanopores graphene membrane*, ChEmference2015 IIT Hyderabad, December 5-6, 2015, Hyderabad, India.
77. Bhandary D, Vasumathi V, MNDS Cordeiro and Singh JK, *Understanding the formation of Janus particles from nano droplets of alkyl thiols*, MRS-Brazil Meeting 2015, October 27-30, 2015, Rio De Janeiro, Brazil.

78. Bhandary D, Benkova Z, Cordeiro MNDS and Singh JK, *Wetting on grafted thermoresponsive polymer brushes: A Molecular Dynamics Study*, Thermodynamics-2015, September 15-18, 2015, Copenhagen, Denmark.
79. Sadanandam S, Nair NN and Singh JK, *A DFT study on the interaction of PMMA polymer chains with ZnS nanoparticle*, Theoretical Chemistry Symposium, December 18-21, 2014, NCL-PUNE, India.
80. K Anitha, Sadanandam N, Singh JK, *Adsorption of heavy metal ions from aqueous media using carbon nanotubes: A molecular dynamics study*, Theoretical Chemistry Symposium, December 18-21, 2014, NCL-PUNE, India.
81. Bhandary D, Singh JK, *Wetting on grafted thermoresponsive polymer brushes: A molecular dynamics study*, 2nd Soft Matter Young Investigators Meeting, December 18-20, 2014, Pondicherry, India.
82. Patra TK, Katiyar P, Singh JK, *Substrate directed self-assembly of anisotropic nanoparticles*, 2nd Soft Matter Young Investigators Meeting, December 18-20, 2014, Pondicherry, India.
83. Bose A, Metya AK and Singh JK, *Effect of electric field on structure and dynamics of nanoconfined water*, Liquids 2014, Lisbon July 21-25, 2014
84. Bhandary D, Srivastava K, Srivastava R and Singh JK, *Effects of electric field on the vapor-liquid equilibria of nanoconfined methanol and ethanol*. ESAT, Eindhoven, July 6-9, 2014
85. Singh JK and Müller-Plathe *Understanding supercooled liquid on nanostructured rough surfaces: A molecular dynamics study*, DPG spring meeting, Regensburg, Germany, March 10-15, 2013
86. Das C and Singh JK, *On the melting of confined Lennard-Jones solids*, AIChE, October 31, 2012, Pittsburg, USA
87. Kumar U, Metya AK and Singh JK, *Study of transport properties and stress analysis using macro and atomistic simulations for lithium based rechargeable batteries*, AIChE, October 31, 2012, Pittsburg, USA
88. Patra TK and Singh JK, *Shape and size effects of nanoparticles on the properties of nanocomposite*. Foundations of Molecular Modeling and Simulation, Portland, USA, July 22-27, 2012.
89. Das C and Singh JK, *On the melting of confined solids*, Foundations of Molecular Modeling and Simulation, Portland, USA, July 22-27, 2012.
90. Patra TK and Singh JK, *Structure and transport of charged polymer over flat and orthogonal surface*, Thermodynamics 2011, Athens, Greece, September 1-3, 2011.

91. Khan S, Singh JK, *Tuning surface phase transition of associating fluid*, Thermodynamics 2011, Athens, Greece, September 1-3, 2011.
92. Srivastava R, Docherty H, Singh JK and Cummings PT, *Phase transition of water in graphite and mica pores*, ESAT 2011, St. Petersburg, Russia, June 25 – 27, 2011.
93. Patra TK and Singh JK, *DNA separation in nano devices*, Chemference 2010, IIT Kanpur, July 13-14, 2010.
94. Khan S and Singh JK, *Self assembled monolayer of n-alkanols on mica surface*, Chemference 2010, IIT Kanpur, July 13 – 14, 2010.
95. Singh SK, Srivastava R and Singh JK, *Phase diagram of fluids confined at nanoscale*, Reach Symposium, IIT Kanpur, India, October 10 – 12, 2010.
96. Khan S, Singh JK, *Phase transitions of associating molecules near active surfaces*, Reach Symposium, IIT Kanpur, October 10 – 12, 2010.
97. Srivastava R, Docherty H, Singh JK and Cummings PT, *Phase transition of water in graphite and mica pores*, AIChE Annual Meeting, Salt Lake City, Utah, U.S.A, November 7 – 12, 2010.
98. Patra TK, Hens A and Singh JK, *Structure, dynamics and phase equilibria of 2D polymeric fluid*, TCS10 (Theoretical Chemistry Symposium), IIT Kanpur, December 8-12, 2010.
99. Mitra S, Ali Sk M, Khan S, Singh JK, *Solvation of Sr<sup>2+</sup> metal ion in different solvents: DFT and MD study*, Theoretical Chemistry Symposium 2010, IIT Kanpur, December 8-12, 2010.
100. Khan S and Singh JK, *Self assembled monolayer of n-alkanols on mica surface: A molecular dynamic study*, 8th Liblice conference, Brno, Czech Republic, June 13-18, 2010.
101. Mitra S, Ali Sk M, Khan S, Tulishetty S and Singh JK, *Solvation of Sr<sup>2+</sup> metal ion in different solvents: DFT and MD study*, 55<sup>th</sup> DAE Solid state Physics Symposium 26, Manipal University, India, December 26 – 30, 2010.
102. Srivastava R, Docherty H, Singh JK and Cummings PT, *Phase transition of water in graphite and mica pores*, 55<sup>th</sup> DAE Solid State Physics Symposium, Manipal University, India, December 26 – 30, 2010.
103. Dutta RC, Khan S and Singh JK, *Wetting transition of water on smooth and texture surface*, PPPEPD, Suzhou, Jiangsu, China, May 16-21, 2010.

104. Singh SK and Singh JK, *Effect of Pore Morphology on Phase Transition and Crossover Behavior*, PPPEPD, Suzhou, Jiangsu, China, May 16-21, 2010.
105. Khan S and Singh JK, *Prewetting of associating fluids near an active surface*, PLMMP 2010, , Kyiv, Ukraine, May 21-24, 2010.
106. Singh SK, Srinivas, MVP, Singh JK, *Design of novel materials for the separation of organic impurities from aqueous medium*, International Conference of Environmental Health and Technology (EH&T 2010) IIT Kanpur, 13th March, 2010.
107. Singh JK, *Fluid Near Surfaces*, Indo-American Frontiers of Engineering, March 10-13, Agra, India 2010.
108. Ghosh A, Singh D, Patra, TK, Singh JK, Gurunath, R, *Electrophoretic Transport of Nucleic Acids through Nanostructured Surfaces*, AIChE Annual Meeting, Nashville, USA, 2009.
109. Singh SK and Singh JK, *Significance of pore size and porosity of mesoporous materials over its surface area for separation of vegetable oil from an aqueous solution*, International Conference on Separation Process, Varanasi, 2009.
110. Bhateja A, Prakash P, Sharam I, Mishra BK and Singh JK, *Three dimensional numerical modeling of horizontal axis planetary mill with variable transmission ratio*, International Seminar on Mineral Processing Technology, Bhubaneswar, 2009.
111. Patra TK and Singh JK, *HPC for designing nano machines and processes*, ATIP symposium on HPC in India, Supercomputing 09, Portland, November 14-20, 2009.
112. Dutta, RC and Singh JK, *Molecular dynamics of nanoscale wetting of water on grooved patterned surfaces*, Asian Particle Symposium, Delhi, 2009.
113. Khan S and Singh JK, *Wetting transition and boundary tension of dimer forming associating fluids*, Asian Particle Symposium, Delhi, 2009.
114. Singh SK and Singh JK *Critical Properties of fluids in nanopores: Crossover from 3D to 2D*. Thermodynamics 2009, Imperial College London, 2009.
115. Singh JK and Singh SK, *Vapor-liquid critical and interfacial properties of semi-flexible chain molecules in nanopores-A molecular modeling study*, Asian Particle Symposium, Delhi, 2009.
116. Singh SK and Singh JK, *Critical Properties of fluids in nanopores: Crossover from 3D to 2D*. AIChE Annual Meeting, Nashville, USA, 2009.

117. Khan S, Kwak SK and Singh JK, *Phase transitions of associating fluids near surfaces*, AIChE Annual Meeting, Nashville, USA, 2009.
118. Huang H, Singh JK and Kwak SK, *Structure and phase behaviours of confined fluids in single walled nanotubes*, AIChE Annual Meeting, Nashville, USA, 2009.
119. Bhateja A, Singh JK, and Sharma I, *Axial segregation in horizontally vibrated granular materials: A numerical study*, International association for computer methods and advances in geomechanics, Goa, 2008.
120. Singh SK, Jana S, Singh JK, *Critical properties of fluids in nanopores*, Chemical engineers congress, Chandigarh, 2008.
121. Singh SK, Jana S, Kwak SK and Singh JK, *Thermophysical properties of confined fluids*, American institute of chemical engineers annual meeting, USA, 2008.
122. Singh JK and Saha A, *Surface phase morphological transitions on functional surfaces*, American institute of chemical engineers annual meeting, USA, 2008.
123. Singh JK, *Wetting transitions on functional surfaces*, Nanomem, FORTH -ICT, Greece, June, 2008.
124. Gazali P, Kwak SK, and Singh JK, *Interface mixing behaviour of Lennard-Jones FCC(100) thin film*, American institute of chemical engineers annual meeting, USA, 2008.
125. Kwak SK, Huang H, and Singh JK, *Structure, fluid-solid coexistence and phase transition of model fluids in cylindrical pore*, American institute of chemical engineers annual meeting, USA, 2008.
126. Singh SK, Singh JK, and Deo G, *Effect of surface characteristics and pore size of nano confinements on the thermophysical properties of natural gas components*, National Conference on Frontiers in Chemical Engineering, IIT Guwahati, 2007.
127. Singh JK, *Phase behaviour, Interfacial properties, structure and dynamics of complex fluid*, Reach IIT Kanpur, 2007.
128. Kanodia R, Agarwal U, Singh JK, *Phase coexistence and Interfacial Properties of simple fluid confined in a disordered porous material.*, International workshop on the physics of mesoscopic and disordered materials, IIT Kanpur, 2006.
129. Kwak SK, Singh JK, Adhikari K, *Vapor-liquid phase coexistence curves for Morse fluids by grand-canonical transition-matrix Monte Carlo simulation*, Regional Symposium on Chemical Engineering, Singapore, 2006.
130. Singh JK, Benjamin KM, and Kofke DA, *Cluster Integral Calculations Via Mayer-Sampling Molecular Simulation: Higher-Order Virial Coefficients, Thermodynamic*

- Properties, and Molecular Clustering*, American Institute of Chemical Engineers, annual meeting, USA, 2005.
131. Kwak SK and Singh JK, *Bulk and Interfacial Properties of Simple Confined Fluids*, American Institute of Chemical Engineers annual meeting, USA, 2005.
  132. Singh JK, Kwak SK and Kofke DA, *Mayer Sampling: Evaluation of Cluster Integrals Using Free-energy Perturbation Methods*, American Institute of Chemical Engineers annual meeting, USA, 2004.
  133. Singh JK and Kofke DA, *Mayer Sampling: Calculation of Cluster Integrals Using Free-energy Perturbation Methods*, Midwest Thermodynamics and Statistical Mechanics Conference, USA, 2004.
  134. Kofke DA, Singh JK, Kwak SK and Di Wu, *Etomica, an API for molecular simulation*, Intl conference on Properties and Phase Equilibria for Product and Process design, Snowbird, Utah, USA, 2004.
  135. Singh JK and Kofke DA, *Molecular simulation study of surface tension of associating fluids: A Monte Carlo Study*, Intl conference on Properties and Phase Equilibria for Product and Process design, Snowbird, Utah, USA, 2004.
  136. Singh JK, Kofke DA, Errington JR and Jones M, *Parallelization of grand-canonical ensemble simulations for Surface Tension Calculation*, American Institute of Chemical Engineers, annual meeting, USA, 2003.
  137. Kofke DA and Singh JK, *Effect of molecular association on vapor-liquid surface tension* ACS Meeting, USA, 2003.
  138. Singh JK and Kofke DA, *Effect of molecular association and solutes on vapor-liquid interfacial properties: A Monte Carlo Study*, American Institute of Chemical Engineers, annual meeting, USA, 2003.
  139. Singh JK and Kofke DA, *Molecular Simulation study of fundamental effects of molecular association on properties of fluid interface*, Foundations of Molecular Modeling and Simulation, Keystone, CO, USA, 2003.
  140. Singh JK, Iacovella CR and Kofke DA *Etomica, an API for molecular simulation*, Foundations of Molecular Modeling and Simulation, Keystone, CO, USA, 2003.
  141. Singh JK and Kofke DA, *Effect of Molecular Association on Interfacial Properties: A Monte Carlo Study*, Midwest Thermodynamics and Statistical Mechanics Conference, USA, 2003.

142. Singh JK, Lu N and Kofke DA *Effecting Monte Carlo Volume changes by localized distortion of space*, American Institute of Chemical Engineers, annual meeting, USA, 2002.
143. Singh JK and Kofke DA, *Molecular Simulation study of fundamental effects of molecular association on properties of fluid interface*, American Institute of Chemical Engineers, annual meeting, USA, 2002.



## RESEARCH SUPERVISION

### (A) Ph. D. Thesis

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

### (B) M.Tech Thesis

1. Vipin Kumar on “ Wettability Alteration due to Low Salinity Waterflooding in Carbonate Reservoir: A Molecular Dynamics Study” 2024
2. Dantuluri Roshini on “A Combined Density Functional Theory and Machine Learning Aided Screening of g-C<sub>3</sub>N<sub>4</sub> Based Single Atom Catalysts for Hydrogen Evolution Reaction” 2023
3. Aindrila Indira on “Understanding the Role of Polymers on the Nucleating Behaviour of Water in Dilute Supercooled Solutions” 2023

4. Priyanka Sinha on “Accelerating the Discovery of 2D Mxenes for Hydrogen Generation using Machine Learning” 2023
5. Ajinkya S Athawale on “Electrochemical Reduction of CO<sub>2</sub> to CH<sub>4</sub> Using Mxene based single atom catalysis” 2023
6. Bavita Kumari on “The role of salts in the recovery of oil: a molecular simulation study” 2022
7. Snehitha Srirangam on “Effect of pressure on ice nucleation under shear” 2022
8. Jaysree Lakela on “Screening of hypothetical zeolites for the separation of hydrogen isotopes” 2022
9. Suraj K on “ Study of confined salt-water at gigapascal high pressure” 2021
10. 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
11. Ashar Ahmad on “Development of a rapid soil testing tool for real time sensing of soil physical and chemical properties” 2020
12. Prantar Dutta on “Drug-Lipid Interactions in Multicomponent Membranes: Insights from Molecular Dynamics Simulations” 2020
13. Tekchand Kumawat on “Development of a portable device for simultaneous determination of soil nutrients” 2019
14. Prerna on “Study of Ice Nucleation on Defective Silver Iodide and Effect of Probing on Dynamics of a Water Droplet” 2019
15. Ankit Srivastava on “Development of a sol-gel membrane for sensing nitrate ions” 2018
16. Sauradeep Majumdar on “Adsorptive Separation of CO<sub>2</sub> from Multicomponent Gas Mixtures in Nanoporous Materials” 2018
17. Chandra Sekhar Sahu on “Development of Handheld Device for Measurement of Micro and Macro Nutrients Concentration in Soil” 2018
18. 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
19. Sandip Charan on “ A Molecular Simulation Study of CO<sub>2</sub> Adsorption using Functionalized and Non- Functionalized CNTs” 2016
20. 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
21. Prasun Haldar on “Selective adsorption of CO<sub>2</sub> using functionalized CMK-5 ordered mesoporous carbon” 2015
22. Akshay Bansal on “Classical density theory for confined polar fluids” 2015
23. Nisha Masawan on “ Experimental investigation on nanoparticle adsorption mechanism on cellulose surface” 2015
24. Aman Sharma on “ Shale gas : adsorption and desorption behavior using molecular simulation” 2014
25. Pooja Sahu on “ Process development for grafting of macrocyclic crown ether on a suitable solid matrix for chromatographic separation of metal ion/isotopes” 2013

26. Utsav Kumar on “Multi-scale simulation of Li-ion battery” 2013
27. Haritha B on “Aqueous solution: adsorption behaviour surfactant/ligand in the presence of heavy metal ions: experiments and simulations” 2013
28. Parul Katiyar on “ Understanding mechanical properties of hollow graphite nanofibers and polyethylene composite: experiments and molecular simulation” 2013
29. Atanu Metya on “ Thermodynamics and transport properties of liquid alkali metals in bulk and near surfaces” 2011
30. Rakesh Kanobodia on “ Structural and transport properties of imidazolium based ionic liquids as electrolytes in li-ion batteries” 2011
31. M. V. P. Srinivas on “ Vapor-liquid phase transition of associating fluids under slit-pore confinement” 2010
32. Ravi C. Dutta on “ Wetting properties of water on smooth and textured surfaces: A molecular dynamics study” 2010
33. Abhiram Hens on “Vapor-liquid phase transition of sodium and 2D polymeric fluids” 2010
34. D. J. Naresh on “ Virial equations of states of simple associating and colloidal fluids: A Monte Carlo Study” 2009
35. Subimal Jana on “ Phase behaviour of square-well fluids in slit pores” 2008
36. A. Naresh on “ Vapor-liquid phase coexistence properties of variable square well fluids and on site associate fluids in repulsive porous media” 2008
37. Rohan Awasti on “ Simulation of Direct Methanol Fuel Cell (DMFC)” 2008
38. 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. Debatra 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- )
28. Dr. M. Aamir Khan (2021-)
29. Dr. Malay Biswal (2022- )
30. Dr. Mayank Gupta (2022-)
31. Dr. Bushnagar Adivaiah (2022-)
32. Dr. Tamaghna Chakraboti (2023-)
33. Dr. Satyabrata Subhodi (2023 )
34. Dr. Sangeeta Mahala (2022-)
35. Dr. Aswathi Mohan (2023-)

**(D) PROJECT ASSOCIATE RESEARCHER: 32**

**SPONSORED PROJECTS (~52 cr INR)**

**(A) GOVERNMENT SPONSORED PROJECTS (Rs. 448 M)**

1. Nature-inspired Insilco design of anti-freeze nanoparticles, SERB, 2024-2027, Rs. 6.6 M
2. R&D of low GWP chemicals, MOEFC, Rs. 5 M
3. CREATE: Centre for rechargeable energy storage system for augmenting transportation and electrification, SERB, 2022-2027 Rs, 84 M
4. DST-BioEnergy and H2 Map, DST,2022-2025, Rs. 11.4 M.
5. Soil health monitoring for agricultural applications, UP-GOVT, 2021-2022, Rs 5.7 M
6. Development of electrochemical biosensors for detection of emerging pollutants in water, DST, 2020-2023, Rs. 6.992 M
7. Structural evaluation of building blocks of ice in different geometry/conditions and its impact on nucleation behaviour, SERB, 2020-2023, Rs. 3.85 million
8. Development of a hybrid approach for high-throughput screening of material, SERB, 2020-2023, Rs. 0.66 million
9. Understanding the self-assembly of amphiphilic molecules in supercooled solvents using molecular simulations, SERB, 2020-2023, Rs. 6.46 million
10. In silico screening for repurposing known drugs for SARS-COV-2 using AI and molecular simulations, SERB, 2020-2021, Rs. 1.669 million
11. One dimensional model for the study of oxidation modeling of PCS fiber on a stationary cylindrical roll, DMSRDE, 2019-2020, Rs. 1.07 million

12. 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.
13. Nucleation of nanostructured surface, DST-RFBR, 2017-2019, Rs. 1.5 million.
14. Boron nitride based adsorbent for removal of arsenic from aqueous streams, DST, 2016-2019, Rs 4.26 million.
15. Wetting behavior of fluids in presence of large particles on surfaces, DST-SERB 2015-2018, Rs 5.93 million.
16. Advanced Computation and Research, MHRD, 2013-2018, Rs 57 million.
17. Adsorption and desorption behavior of nanoparticle on a polymeric surface, CSIR, 2015-2018, Rs. 1.567 million.
18. Center of Material Modeling, Mechanics and Applications, MHRD, 2014-2019, Rs 68.9 million.
19. 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.
20. Molecular simulation study of the wetting behavior of polymer grafted silica surfaces, DST Indo-Portuguese, 2014-2017, Rs. 0.46 million.
21. Segregation of vibrated granular materials, DST 2011-2014, Rs, 3.38 million.
22. Polymer-nanofiber separator for batteries, DST, 2011-2014, Rs 4.14 million.
23. Wetting behaviour of aqueous organic fluids on functional surfaces, UP-CST, 2010-2013, Rs 0.6 million.
24. Molecular simulation of wetting transitions of functional surfaces, CSIR, 2009-2012, Rs 1.2 million.
25. Structural and dynamical properties of organic and aqueous fluids at nanoscale, DST, 2010-2013, Rs 3.35 million.
26. Setting up of a supercomputing facility at IIT Kanpur, DST, 2010-2013, Rs 99.6 million.
27. Improving the wettability of liquid Sodium on Metal/Alloys, DAE-IGCAR, 2009-2011, Rs 1.586 million.
28. Monte Carlo Simulation Study of Metal-Ion Solvent Systems, DAE-BRNS 2009-2012, Rs 3.625 million.
29. Mesoscale Functional Thin Films and Interfaces of Soft Materials, IRPHA, DST, 2007-2011, Rs 49.5 million.
30. Segregation in Heterogeneous Media, IIT Kanpur, 2007-2010, Rs 0.5 million.
31. Molecular simulation of associating fluids and their mixtures. DAE-BRNS, 2006-2009, 1 million.
32. Phase equilibria and interfacial properties of fluid and their mixture in nanoporous materials, DST, New Delhi, 2006-2009, 1.881 million.
33. Structure, dynamics and phase behavior of complex fluids via Molecular Simulation, IIT Kanpur, 2006-2007, 0.9 million.

#### **(B) INDUSTRY SPONSORED PROJECTS (Rs. 81 M)**

1. Effect of water activity and micro surfactant of mixed surfactant system on preservative efficacy, Unilever, 3 M.

2. Development of Indigenous integrated carbon capture and conversion (ICCC) technology, BPCL, 9.996 M
3. Extraction of titanium salts, Nisarg Ispat Pvt. Ltd, 2023, Rs. 3.3 M
4. Technology for health care, SLPL, 2023-2025, Rs. 5.0 million
5. Development of Lab Scale Process for Separation of TIO<sub>2</sub>, Nisarg Ispat Pvt. Ltd, 2022, Rs. 2.6 M
6. Pilot Scale Demonstration of liquid phase sulfonation of aliphatic, alkyl aryl and aromatic alkylates, Technithon Pvt. Ltd., 2022-2024, Rs. 11.3 M
7. Predicting Ion Conductivity and deducing structure-property relationships for hydrated anion exchange membranes using molecular dynamics simulations, Shell, 2022-2025, Rs 9.3 M
8. Project Activities of scientific research in developing portable oral cancer detection device, 2021-2024, LIC HFL, Rs. 10.6 M
9. Development of an interactive cloud based diagnostic platform for oral cancer, Postescap India, 2021-2023, Rs. 3.8 M
10. Impact of humidity and temperature on the structural changes of salt hydrates, Unilever Ltd. 2021-2022, Rs. 1.79 million
11. Phase Diagram of Salt Hydrate in Presence of Surfactant, Unilever Ltd. 2019-2020, Rs. 1.79 million
12. Development of Soil Testing Tool, RTPL, 2019-2020, Rs 1.0 million
13. Predicting the Release of Drugs from Multi-component Supramolecular Membranes, Akimara Biomedicine Pvt. Ltd, 2019-2020, Rs. 1.03 million
14. Martinizing Anti-Cancer Drugs and Optimizing Multi-Component Supramolecular Formulations, Invictus Oncology, 2018-2019, Rs. 1.03 million
15. Research and Development for Chemical Technology, SLPL, 2017-2022, Rs. 7.5 million
16. 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 million
17. Electronic, Optical, Structural and Dynamical Properties of ZnS-PMMA Nanocomposite, Samsung R&D, 2011-2012, Rs 2.50 million
18. Development of extra light and strong anti-weathering nets, Ingen, 2011-12, Rs 0.73 million
19. Understanding adsorption-desorption mechanism of nanoparticles on surfaces, Unilever, 2013-2014, Rs 1.55 million.

## PROFESSIONAL SERVICES

### (A) PROFESSIONAL ACTIVITIES

1. Coordinator of INSA Leadership Development Programme in Science & Technology (LEADS) 2024
2. Coordinator of DST-SATHI meeting, November 4, 2023.
3. Co-Coordinator of INSA Leadership Development Programme in Science & Technology (LEADS) 2023
4. Member of Task force for CCUS (Niti Ayog & Ministry of Steel) 2023
5. Member of DST Task Force for further enhancing infrastructure - 2023
6. Member of the selection committees in IITs, BITS Mesra, NITs and AKTU.
7. Member of PAC for MATRICS -2020
8. Member of National Committee for DST NPDF, ECR, and Chemical and Environmental Engineering PAC (2018-2020)
9. Organising member of LEAP, IIT Kanpur, November 19-30, 2018
10. Session Chair, Computational Method, COMFLU, Roorkee, December 9, 2018
11. Session chair, A discussion meeting on “Recent Advances in Molecular Simulations”, IISc Bangalore, 8-11 February 2018.
12. Organising member, Computational Molecular Engineering, HiPC 2016, Hyderabad, 19 December 2016.
13. Associate Editor, Chemical Engineering Communication, Taylor and Francis, 2016-
14. Session Chair and Organising member of Indo-German Frontiers of Engineering 2015, Agra, February 19-22 2015.
15. Session Chair, European Society of Applied Thermodynamics (ESAT) 2014
16. Session Chair, Current Trends in Theoretical Chemistry, 2013
17. Member of Editorial Board of The Scientific World Journal, 2013-2017
18. Session Chair (Presiding), Foundation of Molecular Modeling and Simulation, Portland, July 22-26, 2012
19. Session Chair, Nanotechnology, National Conference on Frontiers in Chemical Engineering, 2007, IIT G
20. Organizing member of INDO-US conference on Fabronics: Advanced Fabrication, IIT Kanpur, 2010, IIT K
21. Member of high level committee HPC facilities of ministry of earth sciences-2012
22. **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.
23. **External Examiner** for M.Sc. and Ph.D. theses 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. Head, Department of Chemical Engineering           | 2022-2024               |
| 2. Director, IITKDF (section 8 company)               | 2020-2022               |
| 3. Secretary, Alumni Association IIT Kanpur           | 2019-2021               |
| 4. Dean of Resource and Alumni, IIT Kanpur            | 2019-2022               |
| 5. Head, CDTE/QIP                                     | 2018-2019               |
| 6. Nodal Coordinator, National Supercomputing Mission | 2017-2020               |
| 7. HPC Convener                                       | 2016-2020               |
| 8. Associate Dean, UG program                         | 2016-2018               |
| 9. Student Award committee member                     | 2013-2014               |
| 10. S-SAC member                                      | 2011-2012               |
| 11. Treasurer, Alumni Association IIT Kanpur          | 2010-2012               |
| 12. DPGC convener                                     | 2010-2012               |
| 13. DPGC committee member                             | 2008-2010;<br>2013-2014 |
| 14. Warden-in-charge, Hall II                         | 12/2008-05/2009         |
| 15. Chemineer Faculty-in-charge                       | 04/2006-04/2009         |
| 16. Maintenance and Mess Warden, Hall II              | 12/2007-12/2008         |
| 17. CCCC representative                               | 2008                    |
| 18. Faculty Counselor                                 | 2006-2008               |
| 19. Senate AP representative                          | 12/2007-11/2008         |

## **(D) Institutional Building Activities (IIT KANPUR)**



1. Establishment of supercomputing facility
  - 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
2. Founder Director of IITK Development Foundation 2020-2022
  - 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.
  - Revamped the office and automated all the processes
  - Founded another platform, AlmaWorld to bring alumni closer to the institute and to have a reunion platform for ease of operation.
  - Founding member of Gangawal School of Medical Science and Technology
  - Raised funds to create centres ranging from Rozi Siksha Kendra to Center for Neurogenerative diseases.
3. Founding member of Sustainable Energy Engineering 2021
  - a. Created new department and two centres primary focusing on energy engineering along with other members.
4. Established a new Undergraduate Lab of chemical engineering department and Graduate Student Lounge (first in IITK) 2022-23