Curriculum Vitae

Name: Jayant Kumar Singh
Date of Birth: February 03, 1975 (Buxar, Bihar)
Designation: Professor (since June 2015)
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Education

Ph.D. Chemical and Biological Engineering, UB, SUNY at Buffalo, Nov 2004

M.S. Computer Science and Engineering, UB, SUNY at Buffalo, Feb 2002

B.Tech. Chemical Engineering, Indian Institute of Technology Kanpur, May 1997

Awards and Honors

- SERB-STAR AWARD 2020
- Member of Editorial Board, Fluid Phase Equilibria 2020-2022
- Member of EAB, Journal of Chemical Engineering Data 2020-2022
- CSIR-CSMCRI Chemcon Distinguished Speaker Award 2019
- Member of Advisory Board, ACS Omega 2018-2020
- Mr. and Mrs. Gian Singh Bindra Chair Professor 2017-2020
- JSPS Invitation Fellowship 2017
- Associate Editor, Chemical Engineering Communication 2016-2020
- Guest Editor, Special Issue, Molecular Simulation 2014
- Class of 1970 Research Fellowship, IIT Kanpur 2013-2016
- Member of Editorial Board, The Scientific World Journal 2012-2017
- Humboldt Research Fellowship for Experienced Researchers 2012
- Elected as Member, National Academy of Sciences India (NASI) 2011
- Amar Dye-Chem Award, IIChE 2010
- Indian National Academy of Engineering (INAE) Young Engineer Award 2009
- DST-BOYSCAST Fellowship, DST 2008
- IIT Kanpur Reach Symposium Award 2007
- Research Fellow, School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore 2007

- Department of Atomic Energy BRNS Young Scientist Award 2006
- Intl conference on Properties and Phase Equilibria for Product and Process Design support for graduate student 2004
- New York State-GSEU Professional Development Award 2003

Field of Specialization

- Material Modeling
- Statistical mechanics and molecular simulations
- Selective adsorption and separation
- Machine learning

Experience

Dean of Resources and Alumni	July 01, 2019-till date	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 –till date	Department of Chemical Engineering, Indian Institute of Technology, Kanpur, India
Visiting	July 2012-June	Department of Physical Chemistry, Technical

Professor	2013; May-July 2014	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 2012-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 Engineering	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

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* (**Indian Patent Application No:** TEMP/E-1/29007/2019- DEL)

(B) BOOKS

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

(C) OTHER BOOK AUTHORING 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. 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)

4. Singh JK, *Chemical Modeling of Fluids near Surfaces* in *Chemical Modeling*, vol. 8, 72-104, 2017, Royal Society of Chemistry

5. 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)

6. 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).

7. 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).

8. 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).

9. 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).

10. 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 (143, h-index=27)

11. Halder P and Singh JK, High Throughput Screening of Metal-Organic Frameworks for Ethane-Ethylene Separation Using Machine Learning Technique. *Energy & Fuels,* in press, 2020.

12. Namsani S et al, Potential drug candidates for SARS-CoV-2 using computational screening and enhanced sampling methods. *Submitted.*

13. Goswami A, Dalal IS and Singh JK, Seeding Method for Ice Nucleation under Shear. *Accepted*.

14. Yadav VK, Mir S, Mishra V, Gopakumar TG and Singh JK, A Tunable Two-Dimensional Imine Covalent Organic Frameworks as a Platform for Optoelectronic Applications. *Accepted.*

15. Misra V, Mir S, Singh JK and Gopakumar TG, Rationally Designed Semi-Conducting 2D Surface Confined Metal Organic Network. *Accepted.*

16. Maurya M and Singh JK, Selective separation of CO2 from flue gas using carbon and boron nitride nanotubes as a membrane, *Energy & Fuels,* in press, 2020

17. Mir S, Yadav VK and Singh JK, Recent advances in the carrier mobility of two-dimensional materials: a theoretical perspective. *ACS Omega*, in press, 2020

18. 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*, in press, 2020.

19. 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*, in press, 2020

20. Bhangari RS, Yadav VK, Singh JK and Sinha N, "Functionalized Boron Nitride Nanosheets as Novel Adsorbents for Removal of Arsenic(III) from Contaminated Water. *ACS Omega*

21. Goswami R, Goswami A and Singh JK, d-SEAMS: Deferred structural elucidation analysis for molecular simulations, *Journal of Chemical Information and Modeling*, in press, 2020.

22. Kommu A and Singh JK, A review on graphene-based materials for removal of toxic pollutants from wastewater, *Soft Materials,* in press, 2020 (**Invited Article**).

23. 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.

24. 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.

25. 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.

26. 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.

27. Sappidi P and Singh JK, Molecular dynamics study on the adsorption of UO22+ 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**).

28. 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.

29. 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.

30. 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.

31. 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**).

32. 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.

33. 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.

34. 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.

35. 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.

36. 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.

37. 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.

38. 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.

39. 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.

40. 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.

41. 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.

42. Ghosh S and Singh JK, Hydrogen adsorption in pyrindine bridged porphyrin-covalent organic framework, *International Journal of Hydrogen Energy*, 44, 1782-1796, 2019.

43. Metya AK and Singh JK, Ice adhesion mechanism on lubricant-impregnated surfaces using molecular dynamics simulations, *Molecular Simulation*, 45, 394-402, 2019.

44. Sappidi P, Mir SH and Singh JK, Effect of polystyrene length for the extraction of Gd3+ and UO22+ ions using dicyclohexano crown ether (DCH18C6) with octanol and nitrobenzene: A molecular dynamics study, *Journal of Molecular Liquids*, 271, 166-174, 2018.

45. Maurya M and Singh JK, Treatment of flue gas using graphene sponge: A simulation study, *Journal of Physical Chemistry C*. 122, 14654-14664, 2018.

46. 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.

47. Majumdar S, Maurya M and Singh JK, Adsorptive separation of CO_2 from multicomponent mixtures of flue gas in carbon nanotube arrays: A grand canonical Monte Carlo study, *Energy Fuels*, 32, 6090-6097, 2018.

48. Metya A and Singh JK, Nucleation of aqueous salt solutions on solid surfaces, *Journal of Physical Chemistry C*, 122, 8277-8287, 2018.

49. 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, accepted, *Molecular Physics*, 2018.

50. 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.

51. 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.

52. 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.

53. Sappidi PK, Namsani, Ali SM and Singh JK, Extraction of Gd3+ and UO2 2+ 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.

54. 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.

55. Namsani S, Auluck S and Singh JK, Thermal conductivity of thermoelectric material ß-Cu_2Se : Implications on phonon thermal transport**,** *Applied Physics. Letters*, 111,163903 2017.

56. 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.

57. 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.

58. 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.

59. 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.

60. 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.

61. Peng X, Jain S and Singh JK, Separation of N2/CH4/CO2/SO2 gases in disordered carbons obtained using hybrid reverse Monte Carlo simulation, *Journal of Physical Chemistry C*, 121, 13457-13473, 2017.

62. Namsani S, Auluck S, Bhaskar G and Singh JK, An Interaction potential to study the thermal structure evolution of a thermoelectric material: ß-Cu2Se , ,*Journal of Computational Chemistry*, 38, 2161-2170, 2017.

63. Bhateja A, Sharma A and Singh JK, Segregation physics of a macro-scale granular ratchet, *Physical Review Fluids*, 2, 05301 (R), 2017.

64. 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.

65. 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.

66. 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.

67. Maurya M and Singh JK, Capture of SO2 using functionalized bilayer graphene nanoribbons, *Journal of Chemical Physics*, 146, 044704, 2017.

68. Biswal N and Singh JK, Interfacial behavior of nonionic Tween 20 surfactant at oil-water interfaces in the presence of different types of nanoparticles, *RSC Advances*, 113307-113314, 2016.

69. Singh AK and Singh JK, Fabrication of zirconia based durable superhydrophobic–superoleophilic fabrics using non fluorinated materials for oil-water separation and water purification, *RSC Advances*, 6, 103632-103640, 2016.

70. Metya A, Singh JK and Müller-Plathe F, Ice nucleation on nanotextured surfaces: Influence of surface fraction, pillar height and wetting states, *Physical Chemistry Chemical Physics*, 18, 26796-26806, 2016.

71. Biswal NR, Rangera R, and Singh JK, Effect of different surfactants on the interfacial behavior of the n-hexane–water system in the presence of silica nanoparticles, *Journal of Physical Chemistry B*, 120, 7265-7274, 2016.

72. Kommu A, Namsani S, Singh JK, Functionalized nanoporous graphene membrane for heavy metal ion screening, *RSC Advances,* 6, 63190-63199, 2016.

73. Velachi V, Bhandary D, Singh JK and Dias Soeiro Cordeiro MN, Striped gold particles: New insights from molecular dynamics simulations, *Journal of Chemical Physics* 144, 244710, 2016.

74. Halder P, Maurya M, Jain SK and Singh JK, Understanding adsorption of CO2, N2, CH4 and its mixture in functionalized carbon nanopipe array**,** *Physical Chemistry Chemical Physics*, 18, 14007-14016, 2016.

75. Bhateja A,Sharma and Singh JK, Scaling of granular temperature in vibro-fluidized grains *Physics of Fluids* , 28, 043301, 2016.

76. Bhandary D, Benkova Z, Cordeiro MNS and Singh JK, Molecular dynamics study of wetting behavior of grafted thermo-responsive PNIPAAm brushes, *Soft Matter*, 12, 3093-3102, 2016.

77. Yang Y, Rahimi M, Singh JK, Bohem M and Müller-Plathe F, Adsorption and condensation of SO2 in double-walled carbon nanotube arrays studied by Monte Carlo simulations and simple analytical models, *Journal of Physical Chemistry* C, 120, 7510-7521, 2016.

78. Rahimi M, Singh JK and Müller-Plathe F, Adsorption and separation of binary mixtures of SO2, CO2 and N2 by ordered carbon nanotube arrays: Grand-canonical Monte Carlo simulations, *Physical Chemistry Chemical Physics,* 18, 4112-4120, 2016.

79. Katiyar P,Patra TK, Sarkar D, Pramik A and Singh JK, Understanding adsorption behavior of silica nanoparticles over a cellulose surface in an aqueous medium, *Chemical Engineering Science*, 141, 293-303, 2016.

80. Namsani S and Singh JK, Dewetting dynamics of gold film on graphene: Implications for nanoparticle formation, *Faraday Discussion*, 186, 153-170, 2016.

81. Bose A, Metya AK and Singh JK, Surface effect on electromelting behavior of nanoconfined water, *Physical Chemistry Chemical Physics,* 17, 23147-54*,* 2015.

82. Rahimi M, Babu DJ, Singh JK, Yang Y, Schneider JJ and Müller-Plathe F, Double-walled carbon nanotube array for CO2 and SO2 adsorption. *Journal of Chemical Physics,* 143, 124701, 2015.

83. Anitha K, Sada N and Singh JK, Removal of heavy metal ions using functionalized single-walled carbon nanotube: A molecular dynamics study. *Journal of Physical Chemistry A,* 119, 15232, 2015.

84. Singh JK, Guest editorial, *Molecular Simulation*, 41, 361, 2015.

85. Rahimi M, Singh JK and Müller-Plate F, CO2 adsorption on charged carbon nanotube arrays: A possible functional material for electric swing adsorption, *Journal of Physical Chemistry C*,119, 15232-15239, 2015.

86. Sadanandam N, Nisanth NN and Singh JK, Interaction potential models for bulk ZnS, ZnS nanoparticle, and ZnS nanoparticle-PMMA from first-principles, *Journal of Computational Chemistry,* 36, 1176, 2015.

87. Vasumathi V, Bhandary D, Singh JK and Dias Soeiro Cordeiro MN, Structure of mixed self-assembled monolayers on gold nanoparticles at three different arrangements, *Journal of Physical Chemistry C,* 119, 3199–3209, 2015.

88. Sharma A, Sadanandam N and Singh JK, Molecular simulation of shale gas adsorption and diffusion in inorganic nanopores, *Molecular Simulation*, 41, 414-422, 2015.

89. Patra TK, Katiyar P and Singh JK, Substrate directed self-assembly of anisotropic nanoparticles, *Chemical Engineering Science*,121, 16-22, 2015 (**Invited Article**).

90. Ramarez R, Singh JK, Müller-Plate F and Bohm, M, Ice and water droplets on graphite: a comparison of quantum and classical simulations, *Journal of Chemical Physics,* 141, 204701:1-14, 2014 (**Cover Article).**

91. Das CK and Singh JK, Oscillatory melting temperature of stockmayer fluid in slit pores, *Journal of Physical Chemistry C,* 118, 20848-20857, 2014.

92. Das CK and Singh JK, Melting transition of Lennard-Jones fluid in cylindrical pores, *Journal of Chemical Physics,* 140, 204703:1-9, 2014.

93. Bhandary D, Srivastava K, Srivastava R and Singh JK, Effects of electric field on the vapor-liquid equilibria of nanoconfined methanol and ethanol, *Journal of Chemical Engineering Data,* 59, 3090-3097, 2014 (**Invited Article**).

94. Kumar U, Metya AK, Ramakrishnan N and Singh JK, A study of transport properties and stress analysis using atomistic and macro simulations for lithium ion batteries, *Journal of The Electrochemical Society,* 161, A1453-A1460, 2014.

95. Sahu P, Ali MSK and Singh JK, Structural and dynamics aspects of Li^+ ion complexation by dibenzo-18-crown-6(DB18C6) ionophore in pure solvents and at the water-organic interface, *Journal of Molecular Modeling,* 20, 2413:1-12 2014.

96. Patra TK and Singh JK, Localization and stretching of polymer chains at the junction of two surfaces, *Journal of Chemical Physics,* 140, 204909:1-6, 2014.

97. Bhandary D, Khan S and Singh JK, Structure and dynamics of self-assembled monolayer of n-alkanols on a mica surface*, Journal of Physical Chemistry C* 118, 6809-6819, 2014.

98. Metya AK, Khan S and Singh JK, Wetting transition of ethanol-water droplet on smooth and textured surfaces, *Journal of Physical Chemistry C* 118,4113-4121, 2014.

99. Singh JK and Müller-Plathe F, On the characterization of crystallization and ice adhesion on smooth and rough surfaces using molecular dynamics, *Applied Physics Letters,* 104, 021603:1-5, 2014.

100. Patra TK and Singh JK, Polymer directed aggregation and dispersion of anisotropic nanoparticles, *Soft Matter,* 10, 1823-1830, 2014.

101. Khan S and Singh JK, Wetting transition of nanodroplets of water on textured surfaces: a molecular dynamics study, *Molecular Simulation*. 40,458-468, 2014.

102. Das CK and Singh JK, Effect of confinement on the solid-liquid coexistence of Lennard-Jones Fluid, *Journal of Chemical Physics*, 139,174706:1-13, 2013.

103. Rahimi M, Singh JK*, Babu DJ, Schneider JJ and Müller-Plathe F, Understanding carbon dioxide adsorption in carbon nanotube arrays: molecular simulation and adsorption measurements*, Journal of Physical Chemistry C*, 117, 13492−13501, 2013.

104. Patra TK and Singh JK, Coarse-grain molecular dynamics simulations of nanoparticle-polymer melt: Dispersion vs. agglomeration, *Journal Chemical Physics*, 138, 144901:1-7, 2013.

105. Das CK and Singh JK, On the melting transition of Lennard-Jones solids in slit pores, *Theoretical Chemistry Account*, 13, 1351:1-13, 2013.

106. Bhateja A, Sharma I and Singh JK, Axial segregation of horizontally vibrated binary granular mixtures in an offset-Christmas tree channel, *AIP Conference Proceedings*, 105, 1542, 2013.

107. Sharma AK, Khare P, Singh JK and Verma N, Preparation of novel carbon microfiber/carbon nanofiber-dispersed polyvinyl alcohol-based nanocomposite material for lithium-ion electrolyte battery separator, *Materials Science and Engineering C* 33, 1704, 2013.

108. Singh SK and Singh JK, A comparative study of critical temperature estimation of atomic fluid and chain molecules using fourth-order Binder cumulant and simplified scaling laws, *Molecular Simulation*, 39,154, 2013.

109. Singh SP, Singh JK and Sharma A, Adsorption of gas-like molecules to self-aligned square-well fluid channels under confinement of chemically patterned substrates, *Applied Nanoscience,* 3, 179-187, 2013.

110. Patra TK, Hens A and Singh JK, Thermodynamics and transport properties of 2D polymeric fluids, *Journal of Chemical Physics,* 137,0847012: 1-10, 2012.

111. Srivastava R, Cummings PT and Singh JK, Effect of electric field on water confined in graphite and mica pores, *Journal of Physical Chemistry C,* 116, 17594-17603, 2012.

112. Khan S, Bhandary D and Singh JK, Surface phase transition of multiple sites associating fluids, *Molecular Physics*, 110, 1241-1248, 2012.

113. De S, Boda A, Ali SM, Tulishetti S, Khan S and Singh JK, From Microhydration to bulk hydration of Sr2+ metal Ion: DFT and molecular dynamics study, *Journal of Molecular Liquid*, 172, 110-118, 2012.

114. Huang H, Singh JK, Lee JM and Kwak SK, Confining effect of carbon nanotube configuration on phase behavior of hard-sphere fluid, *Fluid Phase Equilibria*, 318, 19-24, 2012.

115. Metya AK, Hens A and Singh JK, Molecular dynamics study of vapor-liquid equilibria and transport properties of Sodium and Lithium based on EAM potentials, *Fluid Phase Equilibria* , 313, 16-24, 2012.

116. Khan S and Singh JK, Surface phase transition of associating fluids on functionalized surfaces, *Journal of Physical Chemistry C,* 115, 17861-17869, 2011.

117. Srivastava R, Dotchery H, Singh JK, and Cummings PT, Phase transition of water in graphite and mica pores, *Journal of Physical Chemistry C*, 115, 12448-12457, 2011.

118. Ghosh A, Patra TK, Rishikant, Singh RK, Singh JK and Bhattacharya S, Surface Electrophoresis of ds-DNA across orthogonal pair of surfaces, *Applied Physics Lett*ers 98,164102:1-3, 2011.

119. Singh SP, Singh JK and Sharma A, Investigating bridge-like structures in a square-well binary mixture using NVT Monte-Carlo simulation, *International Journal of Nanoscience* 10, 329-333, 2011.

120. Singh SK, Khan S, Jana S and Singh JK, Vapour-liquid phase equilibria of square-well fluids in patterned slit pores, *Molecular Simulation* 37,350-360, 2011.

121. Dutta RC, Khan S and Singh JK, Wetting transition of water on graphite and boron-nitride surfaces: a molecular dynamics study, *Fluid Phase Equilibria* 302,310-315, 2011.

122. Singh SK and Singh JK, Effect of pore morphology on vapor–liquid phase transition and crossover behavior of critical properties from 3D to 2D. *Fluid Phase Equilibria*, 300, 182-187, 2011.

123. Singh SK, Kwak SK, Deo G and Singh JK, Phase transition and cross over behavior of colloidal fluids under confinement, *Chemical Physics Letters*, 494, 184-189, 2010.

124. Khan S and Singh JK, Prewetting transition of one site associating fluids, *Journal of Chemical Physics*, **132**, 144501:1-8, 2010.

125. Huang HC, Chen WW, Singh JK and Kwak SK, Direct determination of fluid-solid coexistence of square-well fluids confined in narrow cylindrical hard pores., *Journal of Chemical Physics*. **132**, 224504:1-7, 2010.

126. Singh SK, Saha A and Singh JK, A Molecular simulation study of vapor-liquid critical properties of a simple fluid in attractive slit pores: crossover from 3D to 2D, *Journal of Physical Chemistry B*, **114**, 4283-4292, 2010.

127. Cummings PT, Dotcherty H, Cristopher C, and Singh JK, Phase transition in nanoconfined fluids: The evidence from theory and simulations, *American Institute of Chemical Engineers J*, **56**,842-848, 2010 (**Perspective Article**).

128. Saha AK, Singh SP, Singh JK, and Kwak SK, Quasi-2D and prewetting transition of square-well fluids on a square-well substrate, *Molecular Physics,* **107**, 2189-2200, 2009 .

129. Naresh DJ and Singh JK, Virial coefficients of hard-core attractive Yukawa fluids, *Fluid Phase Equilibria ,* **285,** 36-43, 2009.

130. Singh JK, Suface tension and vapor-liquid phase coexistence of variable range hard-core attractive Yukawa fluids, Frontiers of Molecular Simulation, *Molecular Simulation,* **35**, 880-887, 2009.

131. Jana S, Singh JK and Kwak SK, Vapor-liquid and interfacial properties of square-well fluids in slit pores, *Journal of Chemical Physics,* **130**, 214707:1-8, 2009.

132. Huang HC, Kwak SK and Singh JK, Characterization of fluid-solid phase transition of hard sphere fluids in cylindrical pore via molecular dynamics simulation, *Journal of Chemical Physics*, **130**, 164511:1-6, 2009.

133. Bhateja A, Singh JK, and Sharma I, Axial segregation in horizontally vibrated granular materials: A numerical study, *Korean Journal of Civil Engineering.* **13**, 289-294, 2009.

134. Singh SK, Sinha A, Deo G, and Singh JK, Vapor-liquid phase coexistence, critical properties and surface tension of confined alkanes, *Journal of Physical Chemistry C*, **113**, 7170-7181, 2009.

135. Naresh DJ and Singh JK, Virial coefficient and inversion curve of simple and associating fluids, *Fluid Phase Equilibria,* **279**,47-55, 2009.

136. Gazali P, Kwak SK and Singh JK,Interface mixing behaviour of Lennard-Jones FCC(100) thin film, *Molecular Physics,* **106**, 2417-2423, 2008.

137. Kumar AN and Singh JK, The effects of interaction range, porosity and molecular association on the phase equilibrium of a fluid confined in a disordered porous media. *Molecular Physics*, **106**, 2277-2288, 2008.

138. Kwak SK, Cahyana Y, and Singh JK, Characterization of divacancy in closed packed hard-sphere crystals, *Journal of Chemical Physics*, **128**, 134514:1-6, 2008.

139. Sachdeva S, Ram RP, Singh JK, and Kumar A, Synthesis of Anion Exchange Polystyrene Membranes for the Electrolysis of Sodium Chloride A*merican Institute of Chemical Engineers J,* 5**4**, 940-949, 2008.

140. Singh JK, Sarma G and Kwak SK, Thin-thick surface phase-coexistence and boundary tension of the square-well fluid on a weak attractive surface. *Journal of Chemical Physics*, **128**, 044708: 1-8, 2008.

141. Benjamin KM, Singh JK, Schultz AJ and Kofke DA, Higher order virial coefficients of water models. *Journal of Physical Chemistry B.*, **111**, 11463-11473, 2007.

142. Kwak SK, Singh JK, Adhikar J, Molecular simulation study of vapor-liquid equilibrium of Morse fluids, *Chemical Product and Process Modeling, Berkely Press*, **2**,Article 8, 1-10, 2007.

143. Singh JK, Adhikari J and Kwak SK, Interfacial properties of Morse fluids, *Molecular Physics,* **105**, 981-987, 2007.

144. Singh JK and Kwak SK, Surface tension and vapour-liquid phase coexistence of confined square-well fluid , *Journal of Chemical Physics*, **126**, 024702:1-8, 2007.

145. Singh JK, Adhikari J and Kwak SK, Vapour-liquid phase coexistence curves for Morse fluids, *Fluid Phase Equilibria*, **248**, 1-6, 2006.

146. Singh JK and Errington JR, Calculation of phase coexistence properties and surface tensions of n-alkanes with grand-canonical transition-matrix Monte Carlo simulation and finite-size scaling. *Journal of Physical Chemistry B.*,**110,**1369 - 1376, 2006.

147. Singh JK and Kofke DA, Molecular simulation study of the effect of pressure on the vapor-liquid interface of the square-well fluid. *Langmuir*, **21**, 4218-4226, 2005.

148. Singh JK and Kofke DA, Molecular simulation study of effect of molecular association on vapor-liquid interfacial properties. *Journal of Chemical Physics*, **121**, 9574-9580, 2004.

149. Singh JK and Kofke DA, Molecular simulation study of the vapor-liquid interfacial behavior of a dimer-forming associating fluid, *Molecular Simulation,* **30**, 343-351, 2004.

150. Singh JK and Kofke DA, Mayer sampling: Calculation of cluster integrals using free-energy perturbation methods. *Physical Review Letters*, **92,** 220601:1-4, 2004.

151. Singh JK, Kofke DA and Errington JR, Surface tension and vapor-liquid phase coexistence of the square-well fluid, *Journal Chemical Physics*, **119**, 3405-3412, 2003.

152. Lu N, Singh JK, and Kofke DA, Appropriate methods to combine forward and reverse free-energy perturbation averages, *Journal of Chemical Physics*, **118**, 2977-2984, 2003.

153. 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, 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.

2. Singh JK, Fundamentals of Wetting Transitions, Hindustan Unilever Ltd, April 15, 2020

3. 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

4. Singh JK, Unraveling nanoconfined world using molecular simulations, December 6, COMFLU-2019

5. Singh JK, What nanoparticles can do to bulk and interfacial properties? University of Crete, Greece, May 29, 2019

6. Singh JK, Insights into material behavior via molecular simulations, *Invictus Oncology Pvt. Ltd.* Delhi, October 24, 2018

7. Singh JK, *Fourth industrial revolution,* LEAP, IIT Kanpur, November 20, 2018

8. Singh JK, *Ice nucleation in presence of foreign substances*, Department of Chemistry, TU Darmstadt, June 12, 2018

9. Singh JK, *Ice nucleation in presence of foreign substances,* Department of Chemical and Biological Engineering, NUS, May 21, 2018

10. Singh JK, *Multi-scale simulations of energy materials: some case studies*, Shell India, R&D, April 12, 2018

11. Singh JK, *Phonon thermal transport in β-Cu_2Se using an ab initio derived force-field*, Discussion Meeting on Recent Advances in Molecular Simulations, IISc Bangalore, Febraury 08-11, 2018

12. Singh JK, *Changing world of chemical engineering*, Ujjain Engineering College, 24 March, 2018

13. Singh JK, *Changing world of chemical engineering*, Madan Mohan Malaviya University of Technology, Gorakhpur, Febraury 11, 2018

14. Singh JK, *Molecular insight into nucleation behavior of supercooled water on surfaces.* IMS, Japan, May 18, 2017

15. Singh JK, *What we can learn about nucleation of supercooled water on surfaces using molecular simulatio ?* Okayama University, May 15, 2017

16. Singh JK, Nanoparticles *aggregation and dispersion behaviour, and its effect on thermophysical properties,* Jilin University, October 27, 2016

17. Singh JK, *Molecular insight into fluid behavior near substrate,* Univ Porto, Porto, June 28, 2016

18. Singh JK, *Understanding ice nucleation on nanostructured surfaces,* TU Darmstadt, June 19, 2016

19. Singh JK, *Understanding water behavior on soft/hard surfaces using molecular simulations,* TU Kaiserslautern, May 17, 2016

20. Singh JK, *Molecular insight into fluid behavior near substrate,* IISc Bangalore, April 7, 2016

21. 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

22. Singh JK, *Understanding the formation of Janus particles from nano droplets of alkyl thiols,* Tutzing, Germany, October 21, 2015

23. Singh JK, *Understanding the behavior of supercooled liquid in presence of surfaces using molecular simualtions*, Institute of Thermodynamics, Univ. Stuttgard, Germany, July 07, 2015

24. Singh JK, *Understanding water(ice)-surface behavior*, Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung (IFAM), Bremen, Germany, June 25, 2015

25. Singh JK, *Coarse-grained molecular simulations of nanoparticles and nanocomposites,* BARC, January 16, 2015

26. Singh JK, *Oscillatory behavior of melting behavior of nanoconfined fluids*, TCS 2014, NCL Pune, December 18, 2014

27. Singh JK, *Solid-liquid transition of nanoconfined fluids,* TU Kaiserslautern, Germany, July 15, 2014

28. Singh JK, *Phase transitions of nanoconfined fluids,* SN Bose Institute Kolkatta, April 11, 2014

29. 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

30. Singh JK, *Understanding phase transition at nanoscale: role of external field*, Univ at Porto, 04 December, 2012

31. Singh JK, *Cross over behavior of confined fluids: 3D to 2D,* TU Darmstadt, Germany, July 19, 2012

32. Singh JK, *Phase transitions at nanoscale: role of confinment*, TU Darmstadt, Germany, July 19, 2012

33. Singh JK, *Unveiling thermodynamics at nanoscale*. Planetary Lecture, IIChE Annual Meeting, Annamalai University, December, 2010.

34. Singh JK, *Fluid near surfaces*, Department of Polymer Engineering, BITS Ranchi, January 29, 2010.

35. Singh JK, *Fluid near surfaces*, Department of chemical and biomolecular engineering, Vanderbilt University, November 23, USA, 2009.

36. Singh JK, *Molecular modeling and simulation of fluids near surfaces*, Modeling and simulation of chemical processes, HBTI Kanpur, February, 2009.

37. Singh JK**,** *Molecular modeling and simulation: Can it help in the development of micro and nano devices*?, INDO- US Workshop, IIT Kharagpur, 2009.

38. Singh JK, *Molecular simulation of fluids near surfaces*, HPC workshop, IISc Bangalore, November 2008.

39. Singh JK, *Fluids near surfaces*, Department of Mechanical Engineering, IIT Kanpur, September 2008.

40. Singh JK, *Multi-scale simulation of cluster formation and self Assembly***,** Indo-US workshop, IIT Kanpur , 2007.

41. Singh JK, *Advanced methods for calculating cluster integrals and interfacial properties,* Department of Chemical Engineering, IIT Delhi, 2004.

42. Singh JK, *Advanced methods for calculating cluster integrals and interfacial properties*, Department of Chemical Engineering, IIT Kanpur, 2004.

(G) CONFERENCE PRESENTATIONS

43. 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

44. 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

45. 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

46. Mir SH, Yadav VK and Singh JK, *First principles study of hydrogen evolution reaction on two dimensional boroncarbonnitride in waste-water: a comparative study with graphene and hexagonal boron nitride*, TCS 2019, February 13-16 2019, Bits pilani Rajasthan, India

47. Yadav VK and Singh JK, *First Principle Simulation Study of Two-Dimensional Molecular Films for Opto-Electronic Applications,* 16th Theoretical Chemistry Symposium, February 13-16, 2019, BITS Pilani, India

48. Maurya M and Singh JK, *Sequestration of SO_2/CO_2 from flue gas using Graphene sponge - a simulation study*, Carbon Capture and its utilization, December 14-15, 2018, National Chemical Laboratory, Pune, India

49. Maurya M and Singh JK, *Sequestration of SO_2/CO_2 from flue gas using graphene sponge - a simulation study*, MRS Fall Meeting and Exhibit, Nov 25, 2018, Boston, Massachusetts, USA

50. Metya AK and Singh JK, *Nucleation of aqueous salt solutions on solid surfaces*, Liblice 2018, June17-22, Srni, Czech Republic, 2018

51. Metya AK and Singh JK, *Nucleation of aqueous salt solutions on solid surfaces*, Thermodynamics, September 05-08, Edinburgh, 2017

52. 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

53. Maurya M and Singh JK, *Sequestration of SO_2/CO_2 from flue gas using Graphene sponge - a simulation study, CompFlu,* December 18-20, 2017, IIT Madras, Chennai, India.

54. Namasani S and Singh JK, *Tuning the gold-graphene interface thermal conductance by vacancy defect*s, ICMS, October 23-26, Shanghai, 2016

55. 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.

56. 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

57. 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

58. Namasani S and Singh JK, *Tuning the gold-graphene interface thermal conductance by vacancy defects*, National Materials Day, November 11, IIT Kanpur, 2016, India

59. 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, Instanbul, Turkey.

60. 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.

61. 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.

62. 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.

63. Bhandary D, Benkova Z, Cordeiro MNDS and Singh JK, *Wetting on grafted thermo-responsive polymer brushes: A Molecular Dynamics Study*, Thermodynamics-2015, September 15-18, 2015, Copenhagen, Denmark.

64. 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.

65. 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.

66. 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.

67. 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.

68. 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

69. 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

70. Singh JK and Müller-Plathe *Understanding supercooled liquid on nanostructured rough surfaces: A molecular dynamics study*, DPG spring meeting, Regensburg, Germany, March10-15, 2013

71. Das C and Singh JK, *On the melting of confined Lennard-Jones solids,* AIChE, October 31, 2012, Pittsburg, USA

72. 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

73. 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.

74. Das C and Singh JK, *On the melting of confined solids,* Foundations of Molecular Modeling and Simulation, Portland, USA, July 22-27, 2012.

75. Patra TK and Singh JK, *Structure and transport of charged polymer over flat and orthogonal surface*, Thermodynamics 2011, Athens, Greece, September 1-3, 2011.

76. Khan S, Singh JK, *Tuning surface phase transition of associating fluid*, Thermodynamics 2011, Athens, Greece, September 1-3, 2011.

77. Srivastava R, Docherty H, Singh JK and Cummings PT, *Phase transition of water in graphite and mica pores*, ESAT 2011, St. Petersburg, Russia, June25 – 27 , 2011.

78. Patra TK and Singh JK, *DNA separation in nano devices*, Chemference 2010, IIT Kanpur, July 13-14, 2010.

79. Khan S and Singh JK, *Self assembled monolayer of n-alkanols on mica surface*, Chemference 2010, IIT Kanpur, July 13 – 14, 2010.

80. Singh SK, Srivastava R and Singh JK, *Phase diagram of fluids confined at nanoscale*, Reach Symposium, IIT Kanpur, India, October 10 – 12, 2010.

81. Khan S, Singh JK, *Phase transitions of associating molecules near active surfaces*, Reach Symposium, IIT Kanpur, October 10 – 12, 2010.

82. 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.

83. 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.

84. Mitra S,Ali Sk M, Khan S, Singh JK, *Solvation of Sr2+ metal ion in different solvents: DFT and MD study,* Theoritical Chemistry Symposium 2010, IIT Kanpur, December 8-12, 2010.

85. 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.

86. Mitra S, Ali Sk M, Khan S, Tulishetty S and Singh JK, *Solvation of Sr2+ metal ion in different solvents: DFT and MD study*, 55th DAE Solid state Physics Sysposium 26, Manipal University, India, December 26 – 30, 2010.

87. Srivastava R, Docherty H, Singh JK and Cummings PT, *Phase transition of water in graphite and mica pores*, 55th DAE Solid State Physics Symposium, Manipal University, India, December 26 – 30, 2010.

88. Dutta RC, Khan S and Singh JK, *Wetting transition of water on smooth and texture surface*, PPPEPD, Suzhou,Jiangsu, China, May 16-21, 2010.

89. Singh SK and Singh JK, *Effect of Pore Morphology on Phase Transition and Crossover Behavior*, PPPEPD, Suzhou,Jiangsu, China, May 16-21, 2010.

90. Khan S and Singh JK, *Prewetting of associating fluids near an active surface*, PLMMP 2010, , Kyiv, Ukraine, May 21-24, 2010.

91. 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.

92. Singh JK, *Fluid Near Surfaces*, Indo-American Frontiers of Engineering, March 10-13, Agra, India 2010.

93. Ghosh A, Singh D, Patra, TK, Singh JK, Gurunath, R, *Electrophoretic Transport of Nucleic Acids through Nanostructured Surfaces*, AICHE Annual Meeting, Nashville, USA, 2009.

94. Singh SK and Singh JK, *Significance of pore size and porosity of mesoporous materials over it's surface area for separation of vegetable oil from an aqueous solution,* International Conference on Separation Process, Varanasi, 2009.

95. 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, Bhabaneswar, 2009.

96. 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.

97. Dutta, RC and Singh JK, *Molecular dynamics of nanoscale wetting of water on grooved patterned surfaces*, Asian Particle Symposium, Delhi, 2009.

98. Khan S and Singh JK, *Wetting transition and boundary tension of dimer forming associating fluids*, Asian Particle Symposium, Delhi, 2009.

99. Singh SK and Singh *JK Critical Properties of fluids in nanopores: Crossover from 3D to 2D.* Thermodynamics 2009, Imperial College London, 2009.

100. 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.

101. Singh SK and Singh JK, *Critical Properties of fluids in nanopores: Crossover from 3D to 2D*. AICHE Annual Meeting, Nashville, USA, 2009.

102. Khan S, Kwak SK and Singh JK, *Phase transitions of associating fluids near surfaces*, AICHE Annual Meeting, Nashville, USA, 2009.

103. *Huang H, Singh JK and Kwak SK, Structure and phase behaviours of confined fluids in single walled nanotubes,* AICHE Annual Meeting, Nashville, USA, 2009.

104. 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.

105. Singh SK , Jana S, Singh JK, *Critical properties of fluids in nanopores*, Chemical engineers congress, Chandigarh, 2008.

106. Singh SK, Jana S, Kwak SK and Singh JK, *Thermophysical properties of confined fluids*, American institute of chemical engineers annual meeting, USA, 2008.

107. Singh JK and Saha A, *Surface phase morphological transitions on functional surfaces*, American institute of chemical engineers annual meeting, USA, 2008

108. Singh JK, *Wetting transitions on functional surfaces*, Nanomem, FORTH -ICT, Greece, June, 2008.

109. 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.

110. 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.

111. 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.

112. Singh JK, *Phase behaviour, Interfacial properties, structure and dynamics of complex fluid,* Reach IIT Kanpur, 2007.

113. 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.

114. 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.

115. 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.

116. Kwak SK and Singh JK*, Bulk and Interfacial Properties of Simple Confined Fluids,* American Institute of Chemical Engineers annual meeting,USA, 2005.

117. 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.

118. Singh JK and Kofke DA, *Mayer Sampling: Calculation of Cluster Integrals Using Free-energy Perturbation Methods,* Midwest Thermodynamics and Statistical Mechanics Conference, USA, 2004.

119. Kofke DA, Singh JK, Kwak SKand Di Wu, *Etomica, an API for molecular simulation,* Intl conference on Properties and Phase Equilibria for Product and Process design, Snowbird, Utah, USA, 2004.

120. 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.

121. 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.

122. Kofke DA and Singh JK, *Effect of molecular association on vapor-liquid surface tension* ACS Meeting, USA, 2003.

123. 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.

124. 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.

125. Singh JK, Iacovella CR and Kofke DA *Etomica, an API for molecular simulation,* Foundations of Molecular Modeling and Simulation, Keystone, CO, USA, 2003.

126. Singh JK and Kofke DA*, Effect of Molecular Association on Interfacial Properties: A Monte Carlo Study,* Midwest Thermodynamics and Statistical Mechanics Conference, USA, 2003.

127. 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.

128. 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 SUPERVISON

(A) Ph. D. Thesis

1. Prasad Sonar on "Granular flows over rigid inclined bases that are either spring-supported or externally vibrated" 2019
2. Manish Maurya on "Molecular Simulation Studies on Selective Separation of CO_2/SO_2 from Flue Gas using Porous Materials 2019
3. Parul Katiyar on "Behavior of nanoparticles at interfaces: structure, dynamics and thermodynamic properties" 2018
4. Atanu K. Metya on "Molecular Simulations of Ice Nucleation in the Presence of Foreign Substance" 2018
5. Anitha Kommu on "Removal of Heavy Metal ions and Organic Pollutants from Industrial Wastewater using Nanomaterials" 2017
6. N. Sadanandam on "Force field development and prediction of thermal conductivity of nanocomposites" 2017
7. Debdip Bhandary "Understanding of Self-Assembled Monolayer using Molecular Dynamics Simulations" 2016
8. Ashish Bhateja on "Segregation of granual material: Theory, Experiments and Simulations" 2014
9. Tarak Patra on "Coarse grain molecular modeling of nanoparticle-polymeric system" 2014
10. Chandan Das on "Study of the effects of confinement on melting transition of Lennard-Jones and dipolar fluids" 2014
11. Sandip Khan. on "Wetting transition on patterned surface applications towards nanofluids" 2012
12. Pratima Gazbiyein on "Development of direct alkaline alcohol fuel cell" 2012
13. Sudhir K. Singh on "Phase equilibria and interfacial properties of confined fluids" 2010

(B) M.Tech Thesis

1. Ashar Ahmad on "Development of a rapid soil testing tool for real time sensing of soil physical and chemical properties" 2020
2. Prantar Dutta on "Drug-Lipid Interactions in Multicomponent Membranes: Insights from Molecular Dynamics Simulations" 2020
3. Tekchand Kumawat on "Development of a portable device for simultaneous determination of soil nutrients" 2019
4. Prerna on "Study of Ice Nucleation on Defective Silver Iodide and Effect of Probing on Dynamics of a Water Droplet" 2019
5. Ankit Srivastava on "Development of a sol-gel membrane for sensing nitrate ions 2018
6. Sauradeep Majumdar on "Adsorptive Separation of CO_2 from Multicomponent Gas Mixtures in Nanoporous Materials" 2018
7. Chandra Sekhar Sahu on "Development of Handheld Device for Measurement of Micro and Macro Nutrients Concentration in Soil" 2018

8. 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
9. Sandip Charan on " A Molecular Simulation Study of CO2 Adsorption using Functionalized and Non– Functionalized CNTs" 2016
10. 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
11. Prasoon Haldar on "Selective adsorption of CO2 using functionalized CMK-5 ordered mesoporous carbon" 2015
12. Akshay Bansal on "Classical density theory for confined polar fluids" 2015
13. Nisha Masawan on " Experimental investigation on nanoparticle adsoption mechanism on cellulose surface" 2015
14. Aman Sharma on " Shale gas : adsorption and desorption behavior using molecular simulation" 2014
15. Pooja Sahu on " Process development for grafting of macrocyclic crown ether on a suitable solid matrix for chromatographic separation of metal ion/isotopes" 2013
16. Utsav Kumar on "Multi-scale simulation of Li-ion battery" 2013
17. Haritha B on "Aqueous solution: adsorption behaviour surfactanct/ligand in the presence of heavy metal ions: experiments and simulations" 2013
18. Parul Katiyar on " Understanding mechanical properties of hollow graphite nanofibers and polyethylene composite: experiments and molecular simulation" 2013
19. Atanu Metya on " Thermodynamics and transport properties of liquid alkali metals in bulk and near surfaces" 2011
20. Rakesh Kanobodia on " Structural and transport properties of imidazolium based ionic liquids as electrolytes in li-ion battteries" 2011
21. M. V. P. Srinivas on " Vapor-liquid phase transition of associating fluids under slit-pore confinement" 2010
22. Ravi C. Dutta on " Wetting properties of water on smooth and textured surfaces: A molecular dynamics study" 2010
23. Abhiram Hens on "Vapor-liquid phase transition of sodium and 2D polymeric fluids" 2010
24. D. J. Naresh on " Virial equations of sttes of simple associating and colloidal fluids: A Monte Carlo Study" 2009
25. Subimal Jana on " Phase behaviour of square-well fluids in slit pores" 2008
26. A. Naresh on " Vapor-liquid phase coexistence properties of variable square well fluids and on site associate fluids in repulsive porous media" 2008
27. Rohan Awasti on " Simulation of Direct Methanol Fuel Cell (DMFC)" 2008
28. Ashish Bhateja on " Axial segregation in horizontally vibrated granular material: A numerical study" 2008

(C) POST-DOCTORAL RESEARCHER (21)

- Dr. Satyapal Singh (2009-2010)
- Dr. Rajat Srivastava (2009-2011)
- Dr. Minakshi Sultania (2010-2011)

- Dr. Surendra Jain (2012)
- Dr. Nihar Ranjan Biswal (2015-2017)
- Dr. Ravi Kant (2014-2015)
- Dr. Sarabani Ghosh (2016-2017) (NPDF)
- Dr. Anuj Kumar (2016)
- Dr. Arun K. Singh (2016-2018) (NPDF)
- Dr. Preeti Srivastava (2017-2018)
- Dr. Praveen Sappadi (2017-2019) (NPDF)
- Dr. Shruti Misra (2017-2020) (Young Scientist)
- Dr. Showkat Mir (2018-2020)
- Dr. Vivek Yadav (2018- 2019)
- Dr. Debdip Bhandari (2018-2019)
- Dr. Reema Biswas (2018- 2019)
- Dr. Jyoti Sahu (2019-2020)
- Dr. Debabatra Pramanik (2019-)
- Dr. N. Sadanandam (2019-20)
- Dr. Amit Kumawat (2020)
- Dr. Sujit Das (2020)
- Dr. Moses Abraram (2020-2021)
- Dr. Arpita Srivastava (2020-2021)

(D) PROJECT ASSOCIATE RESEARCHER: 32

SPONSORED PROJECTS

(A) GOVERNMENT SPONSORED PROJECTS (Rs. 339 million)

1. Development of electrochemical biosensors for detection of emerging pollutants in water, DST, 2020-2022, Rs. 6.992 million
2. Structural evaluation of building blocks of ice in different geometry/conditions and its impact on nucleation behaviour, SERB, 2020-2021, Rs. 3.85 million
3. Development of a hybrid approach for high-throughput screening of material, SERB, 2020-2022, Rs. 0.66 million
4. Understanding the self-assembly of amphiphilic molecules in supercooled solvents using molecular simulations, SERB, 2020-2022, Rs. 6.46 million
5. In silico screening for repurposing known drugs for SARS-COV-2 using AI and molecular simulations, SERB, 2020-2021, Rs. 1.669 million
6. One dimensional model for the study of oxidation modeling of PCS fiber on a stationary cylindric roll, DMSRDE, 2019-2020, Rs. 1.07 million
7. Modeling validation and application of ligand coated soft materials for adsorptive separation of GD3+ and UO2+2 ions, DAE-BRNS, 2016-2019, Rs. 4.19 million.
8. Nucleation of nanostructured surface, DST-RFBR, 2017-2019, Rs. 1.5 million.
9. Boron nitride based adsorbent for removal of arsenic from aqueous streams, DST, 2016-2019, Rs 4.26 million.
10. Wetting behavior of fluids in presence of large particles on surfaces, DST-SERB 2015-2018, Rs 5.93 million.
11. Advanced Computation and Research, MHRD, 2013-2018, Rs 57 million.
12. Adsorption and desorption behavior of nanoparticle on a polymeric surface, CSIR, 2015-2018, Rs. 1.567 million.
13. Center of Material Modeling, Mechanics and Applications, MHRD, 2014-2019, Rs 68.9 million.
14. Aligned carbon nanotubes as porous materiasl for selective carbon dioxide adsorption and desorption: effect of pressure and charges, MOES, 2014-2017, Rs. 4.105 million.
15. Molecular simulation study of the wetting behavior of polymer grafted silica surfaces, DST Indo-Portuguese, 2014-2017, Rs. 0.46 million.
16. Segregation of vibrated granular materials, DST 2011-2014, Rs, 3.38 million.
17. Polymer-nanofiber separator for batteries, DST, 2011-2014, Rs 4.14 million.
18. Wetting behaviour of aqueous organic fluids on functinal surfaces, UP-CST, 2010-2013, Rs 0.6 million.
19. Molecular simulation of wetting transitions of functional surfaces, CSIR, 2009-2012, Rs 1.2 million.
20. Structural and dynamical properties of organic and acqueous fluids at nanoscale, DST,2010-2013, Rs 3.35 million.
21. Setting up of a supercomputing facility at IIT Kanpur, DST, 2010-2013, Rs 99.6 million.
22. Improving the wettability of liquid Sodium on Metal/Alloys, DAE-IGCAR, 2009-2011, Rs 1.586 million.

23. Monte Carlo Simulation Study of Metal-Ion Solvent Systems, DAE-BRNS 2009-2012, Rs 3.625 million.
24. Mesostructured Functional Thin Films and Interfaces of Soft Materials, IRPHA, DST, 2007-2011, Rs 49.5 million.
25. Segregation in Heterogeneous Media, IIT Kanpur, 2007-2010, Rs 0.5 million.
26. Molecular simulation of associating fluids and their mixtures. DAE-BRNS, 2006-2009, 1 million.
27. Phase equilibria and interfacial properties of fluid and their mixture in nanoporous materials, DST, New Delhi, 2006-2009, 1.881 million.
28. Structure, dynamics and phase behavior of complex fluids via Molecular Simulation, IIT Kanpur, 2006-2007, 0.9 million.

(B) INDUSTRY SPONSORED PROJECTS (Rs. 18.13 million)

29. Phase Diagram of Salt Hydrate in Presence of Surfactant, Unilever Ltd. 2019-2020, Rs. 1.79 million
30. Development of Soil Testing Tool, RLPL, 2019-2020, Rs 1.0 million
31. Predicting the Release of Drugs from Multi-component Supramolecular Membranes, Akimara Biomedicine Pvt. Ltd, 2019-2020, Rs. 1.03 million
32. Martinizing Anti-Cancer Drugs and Optimizing Multi-Component Supramolecular Formulations, Invictus Oncology, 2018-2019, Rs. 1.03 million
33. Research and Development for Chemical Technology, SLPL, 2017-2021, Rs. 5.4 million
34. 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
35. Electronic, Optical, Structural and Dynamical Properties of ZnS-PMMA Nanocomposite, Samsung R&D, 2011-2012, Rs 2.50 million
36. Development of extra light and strong anti-weathering nets, Ingen, 2011-12, Rs 0.73 million
37. Understanding adsorption-desorption mechanism of nanoparticles on surfaces, Unilever, 2013-2014, Rs 1.55 million.

PROFESSIONAL SERVICES

(A) PROFESSIONAL ACTIVITIES

1. Member of the selection committee in IITs and BITS Mesra
2. Member of PAC for MATRICS -2020
3. Member of National Committee for DST NPDF, ECR, and Chemical and Environmental Engineering PAC (2018-2020)
4. Organising member of LEAP, IIT Kanpur, November 19-30, 2018
5. Sesson Chair, Computational Method, COMFLU, Roorkee, December 9, 2018
6. Session chair, A discussion meeting on "Recent Advances in Molecular Simulations", IISc Bangalore, 8-11 February 2018.
7. Organising member, Computational Molecular Engineering, HiPC 2016, Hyderabad, 19 December 2016.
8. Associate Editor, Chemical Engineering Communication, Taylor and Francis, 2016-
9. Session Chair and Organising member of Indo-German Frontiers of Engineering 2015, Agra, February 19-22 2015.
10. Session Chair, European Society of Applied Thermodynamics (ESAT) 2014
11. Session Chair, Current Trends in Theoretical Chemistry, 2013
12. Member of Editorial Board of The Scientific World Journal, 2013-2017
13. Session Chair (Presiding), Foundation of Molecular Modeling and Simulation, Portland, July 22-26, 2012
14. Session Chair, Nanotechnology, National Conference on Frontiers in Chemical Engineering, 2007, IIT G
15. Organizing member of INDO-US conference on Fabrionics: Advanced Fabrication, IIT Kanpur, 2010, IIT K
16. Member of high level committee HPC facilities of ministry of earth sciences.
17. **Reviewer** for Phys. Rev. Letts.; Langmuir; J. Chem. Phy.; 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.
18. **External Examiner** for M.Sc. and Ph.D. theses of Queensland University, Indian Institute of Science, Bangalore, Indian Institute of Technology Madras, Indian Institute of Technology Guwahati, Indian Institute of Technology Kharagpur, Indian Institute of Technology Bombay,

(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.	Dean of Resource and Alumni, IIT Kanpur	2019-2022
2.	Head, CDTE/QIP	2018-2019
3.	Nodal Coordinator, National Supercomputing Mission	2017-2020
4.	HPC Convener	2016-
5.	Associate Dean, UG program	2016-2018
6.	Student Award committee member	2013-2014
7.	S-SAC member	2011-2012
8.	Treasurer, IIT K Alumni Association	2010-2012
9.	DPGC convener	2010-2012
10.	DPGC committee member	2008-2010; 2013-2014
11.	Warden-in-charge, Hall II	12/2008-05/2009
12.	Chemineer Faculty-in-charge	04/2006-04/2009
13.	Maintenance and Mess Warden, Hall II	12/2007-12/2008
14.	CCCC representative	2008
15.	Faculty Counselor	2006-2008
16.	Senate AP representative	12/2007-11/2008