Curriculum Vitae

Name: Jayant Kumar Singh
Date of Birth: February 03, 1975 (Buxar, Bihar)
Designation: Professor (since June 2015)
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
Web: http://www.iitk.ac.in/che/jks.htm

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

- Member of Editorial 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-till date
- 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

- Thermodynamics
- Statistical mechanics and molecular simulations
- Confined fuids and fluids at interfaces
- Phase transitions
- Selective adsorption and separation

Experience

Visiting Professor	May 2017	Department of Chemistry, Okayama University, Japan
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 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 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)

(B) BOOKS

1. Singh JK and Verma N, *Aqueous Phase Adsorption: Theory, Simulations and Experiments*, CRC Press (2018)

(C) OTHER BOOK AUTHORING ACTIVITIES

1. 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

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

2. 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)

3. 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).

4. 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).

5. 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).

6. 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).

7. 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

8. 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, Mol. Phy. (2018)

9. 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

10. 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

11. 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

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

13. 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

14. 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

15. 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

16. 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

17. 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

18. 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

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

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

21. 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

22. 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

23. 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

24. Maurya M and Singh JK, Capture of SO2 using functionalized bilayer Graphene Nanoribbons, *Journal of Chemical Physics*, 146, 044704, 2017

25. 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

26. 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

27. 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

28. 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

29. Kommu A, Namsani S, Singh JK Functionalized Nanoporous Graphene Membrane for Heavy Metal Ion Screening, *RSC Advances,* 6, 63190-63199, 2016

30. 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

31. 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

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

33. 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

34. 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

35. 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

36. 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

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

38. Bose A, Metya AK and Singh JK, Surface Effect on Electromelting Behavior of Nanoconfined Water, *Physical Chemistry Chemical Physics,* 17, 23147-54, 2015

39. 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

40. 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

41. Singh JK, Guest Editorial *Molecular Simulation*, 41, 361, 2015

42. 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

43. 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

44. 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

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

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

47. 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)**

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

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

50. 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**)

51. 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

52. 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

53. 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

54. 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

55. 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

56. 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

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

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

59. 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

60. 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

61. 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

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

63. 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.

64. 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.

65. 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

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

67. 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.

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

69. 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.

70. 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.

71. 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.

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

73. 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.

74. 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.

75. 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.

76. 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.

77. 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.

78. 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.

79. 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.

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

81. 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.

82. 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.

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

84. 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 .

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

86. 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.

87. 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.

88. 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.

89. 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.

90. 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.

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

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

93. 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.

94. 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.

95. 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.

96. 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.

97. 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.

98. 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.

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

100. 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.

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

102. 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.

103. 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.

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105. 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.

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

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

108. 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.

109. 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, *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

2. Singh JK, *Changing World of Chemical Engineering*, Madan Mohan Malaviya University of Technology, Gorakhpur, Feb 11, 2018

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

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

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

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

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

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

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

10. 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

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

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

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

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

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

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

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

18. 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

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

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

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

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

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

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

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

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

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

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

29. Singh JK, *Multi-scaleMulti-scale simulation of Cluster formation and Self Assembly***,** Indo-US workshop, IIT Kanpur , 2007.

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

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

(G) CONFERENCE PRESENTATIONS

32. Atanu K Metya and Jayant K Singh, *Nucleation of Aqueous Salt Solutions on Solid Surfaces*, Thermodynamics, September 05-08, Edinburgh, 2017

33. Parul Katiyar and Jayant K Singh, *A coarse-grain molecular dynamics study of oil–water interfaces in the presence of silica nanoparticles and nonionic surfactants*, September 05-08, Edinburgh, 2017

34. Sadanandam Namasani and Jayant K Singh, *Tuning the gold-graphene interface thermal conductance by vacancy defect*s, ICMS, October 23-26, Shanghai, 2016

35. K Anitha and Jayant K singh, *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.

36. Parul Katiyar and Jayant K Singh, *Understanding adsorption behavior of silica nanoparticles over a cellulose surface in an aqueous medium*, Faraday Discussion, February 6-9, 2016, IIT Mumbai, India.

37. K Anitha, Sadanandam Namasani and Jayant K Singh, Molecular Dynamics Simulations of Heavy Metal Ion Rejection Through Functionalized Nanopores Graphene Membrane, ChEmference2015 IIT Hyderabad, December 5-6, 2015, Hyderabad, India

38. Sadanandam Namasani and Jayant K Singh, *Tuning the gold-graphene interface thermal conductance by vacancy defects*, National Materials Day, November 11, IIT Kanpur, 2016

39. Bhandary D, Benkova Z, Cordeiro MNDS and JK Singh*, Wetting Behaviour of Grafted Thermoresponsive PNIPAAm Brushes: A Molecular Dynamics Study*, APMAS2016 1-3 June, 2016, Instanbul, Turkey.

40. Parul Katiyar and Jayant K Singh, *Understanding adsorption behavior of silica nanoparticles over a cellulose surface in an aqueous medium*, Faraday Discussion, February 6-9, 2016, IIT Mumbai, India.

41. K Anitha, Sadanandam Namasani and Jayant K Singh, *Molecular Dynamics Simulations of Heavy Metal Ion Rejection Through Functionalized Nanopores*

Graphene Membrane, ChEmference2015 IIT Hyderabad, December 5-6, 2015, Hyderabad, India.

42. Bhandary D, Vasumathi V, MNDS Cordeiro and Jayant K Singh, *Understanding the formation of Janus particles from Nano Droplets of Alkyl Thiols*, MRS-Brazil Meeting 2015, October 27-30, 2015, Rio De Janeiro, Brazil.

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

44. 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.

45. 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.

46. 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.

47. 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.

48. 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

49. 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

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

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

52. 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

53. 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.

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

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

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

57. 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.

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

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

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

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

62. 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.

63. 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.

64. 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.

65. 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.

66. 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.

67. 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.

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

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

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

71. 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.

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

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

74. 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.

75. 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.

76. 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.

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

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

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

80. 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.

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

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

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

84. 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.

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

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

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

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

89. 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.

90. 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.

91. 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.

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

93. 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.

94. 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.

95. 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.

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

97. 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.

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

99. 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.

100. 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.

101. 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.

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

103. 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.

104. 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.

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

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

107. 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.

108. 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. Atanu K. Metya on "Molecular Simulations of Ice Nucleation in the Presence of Foreign Substance" 2018
2. Anitha Kommu on " Removal of Heavy Metal ions and Organic Pollutants from Industrial Wastewater using Nanomaterials" 2017
3. N. Sadanandam on "Force field development and prediction of thermal conductivity of nanocomposites" 2017
4. Debdip Bhandary "Understanding of Self-Assembled Monolayer using Molecular Dynamics Simulations" 2016
5. Ashish Bhateja on "Segregation of granual material: Theory, Experiments and Simulations" 2014
6. Tarak Patra on " Coarse grain molecular modeling of nanoparticle-polymeric system" 2014
7. Chandan Das on "Study of the effects of confinement on melting transition of Lennard-Jones and dipolar fluids" 2014
8. Sandip Khan. on "Wetting transition on patterned surface applications towards nanofluids" 2012
9. Pratima Gazbiyein on " Development of direct alkaline alcohol fuel cell" 2012
10. Sudhir K. Singh on " Phase equilibria and interfacial properties of confined fluids" 2010

(B) M.Tech Thesis

1. 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
2. Sandip Charan on " A Molecular Simulation Study of CO2 Adsorption using Functionalized and Non– Functionalized CNTs" 2016
3. 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
4. Prasoon Haldar on "Selective adsorption of CO2 using functionalized CMK-5 ordered mesoporous carbon" 2015
5. Akshay Bansal on "Classical density theory for confined polar fluids" 2015
6. Nisha Masawan on " Experimental investigation on nanoparticle adsoption mechanism on cellulose surface" 2015
7. Aman Sharma on " Shale gas : adsorption and desorption behavior using molecular simulation" 2014
8. Pooja Sahu on " Process development for grafting of macrocyclic crown ether on a suitable solid matrix for chromatographic separation of metal ion/isotopes" 2013
9. Utsav Kumar on "Multi-scale simulation of Li-ion battery" 2013
10. Haritha B on "Aqueous solution: adsorption behaviour surfactanct/ligand in the presence of heavy metal ions: experiments and simulations" 2013

11. Parul Katiyar on " Understanding mechanical properties of hollow graphite nanofibers and polyethylene composite: experiments and molecular simulation" 2013
12. Atanu Metya on " Thermodynamics and transport properties of liquid alkali metals in bulk and near surfaces" 2011
13. Rakesh Kanobodia on " Structural and transport properties of imidazolium based ionic liquids as electrolytes in li-ion battteries" 2011
14. M. V. P. Srinivas on " Vapor-liquid phase transition of associating fluids under slit-pore confinement" 2010
15. Ravi C. Dutta on " Wetting properties of water on smooth and textured surfaces: A molecular dynamics study" 2010
16. Abhiram Hens on "Vapor-liquid phase transition of sodium and 2D polymeric fluids" 2010
17. D. J. Naresh on " Virial equations of sttes of simple associating and colloidal fluids: A Monte Carlo Study" 2009
18. Subimal Jana on " Phase behaviour of square-well fluids in slit pores" 2008
19. A. Naresh on " Vapor-liquid phase coexistence properties of variable square well fluids and on site associate fluids in repulsive porous media" 2008
20. Rohan Awasti on " Simulation of Direct Methanol Fuel Cell (DMFC)" 2008
21. Ashish Bhateja on " Axial segregation in horizontally vibrated granular material: A numerical study" 2008

(C) POST-DOCTORAL RESEARCHER: 10
(D) PROJECT ASSOCIATE RESEARCHER: 30

SPONSORED PROJECTS

(A) GOVERNMENT SPONSORED PROJECTS

1. 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 millions
2. Boron nitride based adsorbent for removal of arsenic from aqueous streams, DST, 2016-2019, Rs 4.26 millions
3. Wetting behavior of fluids in presence of large particles on surfaces,DST-SERB 2015-2018, Rs 5.93 millions
4. Advanced Computation and Research, MHRD, 2013-2018, Rs 57 millions
5. Adsorption and desorption behavior of nanoparticle on a polymeric surface, CSIR, Rs. 1.567 millions, 2015-2018
6. Center of Material Modeling, Mechanics and Applications, MHRD, 2014-2019, Rs 68.9 millions
7. Aligned carbon nanotubes as porous materiasl for selective carbon dioxide adsorption and desorption: effect of pressure and charges, MOES, 2014-2017, Rs. 4.105 millions
8. Molecular simulation study of the wetting behavior of polymer grafted silica surfaces, DST Indo-Portuguese, 2014-2017, Rs. 0.46 millions
9. Segregation of vibrated granular materials, DST 2011-2014, Rs, 3.38 millions
10. Polymer-nanofiber separator for batteries, DST, 2011-2014, Rs 4.14 millions
11. Wetting behaviour of aqueous organic fluids on functinal surfaces, UP-CST, 2010-2013, Rs 0.6 millions
12. Molecular simulation of wetting transitions of functional surfaces, CSIR, 2009-2012, Rs 1.2 millions.
13. Structural and dynamical properties of organic and acqueous fluids at nanoscale, DST,2010-2013,Rs 3.35 millions.
14. Setting up of a supercomputing facilty at IIT Kanpur, DST, 2010-2013, Rs 99.6 millions.
15. Improving the wettability of liquid Sodium on Metal/Alloys, DAE-IGCAR, 2009-2011, Rs 1.586 millions.
16. Monte Carlo Simulation Study of Metal-Ion Solvent Systems, DAE-BRNS 2009-2012, Rs 3.625 millions.
17. Mesostructured Functional Thin Films and Interfaces of Soft Materials, IRPHA, DST, 2007-2011, Rs 49.5 millions.
18. Segregation in Heterogeneous Media, IIT Kanpur, 2007-2010, Rs 0.5 million.
19. Molecular simulation of associating fluids and their mixtures. DAE-BRNS, 2006-2009, 1 million.
20. Phase equilibria and interfacial properties of fluid and their mixture in nanoporous materials, DST, New Delhi, 2006-2009, 1.881 millions.
21. Structure, dynamics and phase behavior of complex fluids via Molecular Simulation, IIT Kanpur, 2006-2007, 0.9 million.

(B) INDUSTRY SPONORED PROJECTS

22. Research and Development for Chemical Technology, SLPL, 2017-2019, Rs. 0.21 millions
23. 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 millions
24. Electronic, Optical, Structural and Dynamical Properties of ZnS-PMMA Nanocomposite, Samsung R&D, 2011-2012, Rs 2.50 millions
25. Development of extra light and strong anti-weathering nets, Ingen, 2011-12, Rs 0.73 million
26. Understanding adsorption-desorption mechanism of nanoparticles on surfaces, Unilever, 2013-2014, Rs 1.55 million.

PROFESSIONAL SERVICES

(A) PROFESSIONAL ACTIVITIES

1. Session chair, A discussion meeting on "Recent Advances in Molecular Simulations", IISc Bangalore, 8-11 February 2018.
2. Organising member, Computational Molecular Engineering, HiPC 2016, Hyderabad, 19 December 2016.
3. Associate Editor, Chemical Engineering Communication, Taylor and Francis, 2016-
4. Session Chair and Organising member of Indo-German Frontiers of Engineering 2015, Agra, February 19-22 2015.
5. Session Chair, European Society of Applied Thermodynamics (ESAT) 2014
6. Session Chair, Current Trends in Theoretical Chemistry, 2013
7. Member of Editorial Board of The Scientific World Journal, 2013-2017
8. Session Chair (Presiding), Foundation of Molecular Modeling and Simulation, Portland, July 22-26, 2012
9. Session Chair, Nanotechnology, National Conference on Frontiers in Chemical Engineering, 2007, IIT G
10. Organizing member of INDO-US conference on Fabrionics: Advanced Fabrication, IIT Kanpur, 2010, IIT K
11. Member of high level committee HPC facilities of ministry of earth sciences.
12. **Nodal Coordinator**, National Supercomputing Mission.
13. **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.
14. **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. Convener SERC School-cum-Symposium on molecular simulation November 27-30, 2012
2. Delivered a lecture in Molecular Modeling workshop at UICT, Mumbai, Jan, 2012.
3. Delivered a lecture in ICTS School on "Understanding Molecular Simulations: Theory and Applications" UMS(2010) held at IIT Kanpur during November 4-13, 2010.

4. Delivered a lecture in SERC School on Molecular Simulations for Chemical engineers, IISc Bangalore, May, 2009

(C) ADMINISTRATIVE SERVICES (IIT KANPUR)

1.	HPC Convener	2016-
2.	Associate Dean, UG program	2016-2018
3.	Student Award committee member	2013-2014
4.	S-SAC member	2011-2012
5.	Treasurer, IIT K Alumni Association	2010-2012
6.	DPGC convener	2010-2012
7.	DPGC committee member	2008-2010; 2013-2014
8.	Warden-in-charge, Hall II	12/2008-05/2009
9.	Chemineer Faculty-in-charge	04/2006-04/2009
10.	Maintenance and Mess Warden, Hall II	12/2007-12/2008
11.	CCCC representative	2008
12.	Faculty Counselor	2006-2008
13.	Senate AP representative	12/2007-11/2008