Curriculum-Vitae

Name: Jagannath Mondal
Date of Birth: 17/03/1983
Current Position: Associate Professor

Full Correspondence Address

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Work experience (In reverse chronological order)

- **Associate Professor** Tata Institute of Fundamental Research, Hyderabad India July 2021-Present
- **Reader (F)** at Tata Institute of Fundamental Research, Hyderabad India July 2016-June 2021
- **Reader (E)** at Tata Institute of Fundamental Research, Hyderabad India June 2015-June 2016
- **Postdoctoral Associate** (with **Bruce J. Berne**)at Columbia University, New York, October 2011-June 2015

Academic Qualification (In reverse chronological order)

- Ph. D. at University of Wisconsin Madison, USA (**Advisor: Arun Yethiraj**) September 2011
- M. Sc. in Chemistry at Indian Institute of Technology, Kanpur, 2006
- B. Sc in Chemistry at Calcutta University, 2004

Details of PhD

- Thesis Title: **"Multiscale simulation of amphiphilic macromolecules"**
- Supervisor: Professor Arun Yethiraj
- University: **University of Wisconsin Madison, USA**
- **Year of Award: September, 2011**

Professional recognition/Award/Fellowship

- Award of Alexander von Humboldt fellowship for experienced researcher (2024-2026)

- Induction to Editorial Advisory Board Member of Journal of Physical Chemistry (2024-2027)
- Chemical Research Society of India (CRSI) Bronze medal Award for 2024
- TIFR-Infosys Leading edge grant awardee 2022
- Associate of Indian Academy of Sciences 2016-2019
- Ramanujan Fellowship 2015-2020
- Hirschfelder Prize at University of Wisconsin Madison 2006
- Rank 1 in Calcutta University based on B. Sc. Chemistry examination 2004

Key Research Directions

- Theory and Computer Simulation of Chemically and Biologically relevant Processes
- Computer simulation of biomolecular recognition processes and Drug Discovery
- Molecular Dynamics simulation of protein folding and interaction of osmolytes
- Computer Simulation of Biological membrane and its interaction with protein
- Integrative modelling of sub-cellular organization of bacterial and eukaryotic cytoplasm
- Modelling Materials science and electrocatalytic reaction
- Modelling transport across supramolecular assembly

Brief Research Accomplishments

1. Precise elucidation of biomolecular recognition at atomic scale and in real time:

   Dr. Jagannath Mondal's research has been able to make outstanding progress in capturing protein-ligand binding processes at an atomistic precision in real time via Molecular Dynamics simulation. The initiative has been successful in elucidating substrate-recognition pathways in multiple complex systems (J.Am.Chem.Soc. (2023), JACS Au (2023), J.Am.Chem. Soc.(2018), 140,17743 and J.Biol. Chem. (2021), 297,101271), hitherto inaccessible in experiment. His research has provided promising computational breakthrough for affordable simulation of dynamical recognition processes via coarse-grained computer model (J.Phys.Chem. Lett. (2020), 11,5302). These novel directions are first of its kind in India and provide fresh perspectives. Dr. Mondal serves as the corresponding author in all the work related to this project.

2. Dissection of mechanistic role of osmolytes on stabilization of macromolecules:

   The research group has addressed multiple intriguing questions pertaining to mechanistic role of protein-stabilizing osmolytes under salt and cold-stress via free energy based computer simulation and statistical mechanics (J.Phys.Chem. Lett. (2022), J.Phys.Chem. (2021), J.Phys.Chem.B (2019), J.Phys.Chem.B (2019), J.Phys.Chem.B (2018)). Many of the investigations started out as computer simulation but subsequently got validations via design of judicious experiments (2023). As a key achievement, a set of articles, in each of which Dr. Mondal is the corresponding author, have recently been highlighted by Journal of Physical Chemistry B in a special virtual issue on osmolyte and crowders.

3. Quantifying Conformational reaction coordinate of Biomolecules via Machine Learning:

   A key accomplishment of Dr. Mondal's research as a PI has been the derivation of suitable reaction coordinate for quantifying energy landscape of large biomolecules. Dr. Mondal has been successful in resolving the kinetic pathway of folding of a flexible protein via statistical models (J.Chem.Phys. (2018)). The resulting publication, in which the nominee is the corresponding author, had been selected as feature article by the journal. Last few years. Dr. Mondal has also contributed to design of Machine-learning based approaches as novel scheme of optimization of reaction coordinate as well as utilizing them to identify key metastable states in protein and protein-substrate complex (J.Chem.Phys. (2021)), J.Chem. Phys. (2023), J.Phys.Chem.(2023). He has also started new avenues in using Machine-learning based classification approaches to identify unique conformations for specific functions (J.Chem. Theory Comput.(2023)

4. Towards whole-cell simulation of living bacteria:

   Dr. Mondal has recently led his team to put forth a computer model of cell-interior of bacteria. Specifically, his team has combined theoretical chemistry with experimentally derived data and has come up with a model of bacteria's chromosome. The investigation has recently been published in Nucleic Acids Research (NAR), a high impact journal (IF 16) (NAR (2021), 49,3077) and have initiated exciting new avenue in his group. This has been followed up by multiple extensive works (Phys. Rev. E. (2022), Biophys.J.(2023), J.Chem.Theory Comput.(2023)

5. Fostering Collaboration with experimentalists:

   Apart from leading independent research as a PI , Dr. Mondal's group has also fostered successful collaborations with numerous experimentalists in India and has provided crucial insights needed for understanding new observations or designing new molecules. (Nature Communications (2023, in press), J.Am. Chem. Soc. (2023), Nano Letter (2022), Chemical. Science (2021), Chemical. Science. (2022a, 2022b), Science. Advances (2020), ACS catalysis (2022), ACS Biomater. Sci. Eng. (2019), Phys.Chem.Chem.Phys.(2018), Nature Communications.(2019), J.Biol.Chem.(2017))

Summary of Research output

- Total number of publications in peer-reviewed journal: **99**
- Number of publications in independent career at TIFR-H (June 2015-present): **79**
- Number of Publications in current associate professor position (July 2021-Present): **44**
- Number of PhD students graduated: **6**
- Number of postdoctoral fellows graduated: **4**
- Current number of PhD students: **7**
- Current number of postdoctoral fellows: **2**

Publications (Five most important papers highlighted)

A. As Principal Investigator (July 2015-present)

(* : As Corresponding author)

A1. Since Promotion to Associate Professor (July 2021-present)

99. A. Wasim, S. Menon and **J. Mondal*** "Modulation of alpha-Synuclein Aggregation Amid Diverse Environmental Perturbation" *elife* 13,RP95180 (**2024)**

98. R. Sharma, S. Sarkar, S. Chattopadhyay, **J. Mondal*** and P. Talukdar* "A Halogen-Bond-Driven Artificial Chloride-Selective Channel Constructed from 5-Iodoisophthalamide-based Molecules" *Angew. Chem. Int. Ed.* in press, (**2024)**

97. A. Wasim, P. Bera and **J. Mondal*** "Elucidation of Spatial Positioning of Ribosomes around Chromosome in Escherichia coli Cytoplasm via a Data-Informed Polymer-Based Model" *J. Phys. Chem. B* in press, (**2024)**

96. A. Wasim, P. Bera and **J. Mondal*** "Development of a Data-Driven Integrative Model of a Bacterial Chromosome" *J. Chem. Theory Comput.* 20, 1673 (**2024)**

95. S. Sarkar, T. N. Narayanan **J. Mondal*** "A Synergistic View on Osmolytes Role Against Salt and Cold Stress in Bio-interfaces" *Langmuir* 49, 17581,(**2023)**

94. S. Adhikari and **J. Mondal*** "Machine Learning Subtle Conformational Change due to Phosphorylation in Intrinsically Disordered Proteins" *J. Phys. Chem. B.* 127, 9433,(**2023)**

93. M. Sahil, T. Singh, S. Ghosh and **J. Mondal*** "3site Multisubstrate-Bound State of Cytochrome P450cam" *J. Am. Chem. Soc.* 145, 23488,(**2023)**

92. M. Sahil, J. Singh, S. Sahu, S. K. Pal, A. Yadav, R. Anand and **J. Mondal*** "Identifying Selectivity Filters in Protein Biosensor for Ligand Screening" *JACS Au* 3, 2800,(**2023)**

91. S. Sarkar, A. Guha, R. Sadhukhan, T. N. Narayanan and **J. Mondal*** "Osmolytes as Cryoprotectants under Salt Stress" *ACS Biomater. Sci. Eng.* 9, 5639,(**2023)**

90. B. Dandekar, B. B. Majumdar and **J. Mondal*** "Nonmonotonic Modulation of the ProteinLigand Recognition Event by Inert Crowders" *J. Phys. Chem. B* 9, 7449,(**2023)**

89. C. Ghosh, S. Menon, S. Ball, S. Goswami, **J. Mondal**, D. Das "Emergence of Catalytic Triad by Short Peptide Based Nanofibrillar Assemblies" *Nano Lett.* 23, 5828,(**2023)**

88. B. Dandekar, N. Ahalawat, S. Sinha and **J. Mondal*** "Markov State Models Reconcile Conformational Plasticity of GTPase with Its Substrate Binding Event" *JACS Au* 3, 1728,(**2023)**

87. S. Bandyopadhyay and **J. Mondal*** "A deep encoderdecoder framework for identifying distinct ligand binding pathways" *J. Chem. Phys.* 158, 194103 (**2023)**

86. K. D. Tulsiyan, A. Mahalik, B. Dandekar, **J. Mondal*** and H. S. Biswal "Enhancement of Peroxidase Activity in Magnetic Ionic Liquids" *ACS Sustainable Chemistry Engineering* 11, 8487 (**2023)**

85. S. Menon and **J. Mondal*** "Conformational Plasticity in alpha-Synuclein and How Crowded Environment Modulates It" *J. Phys. Chem. B* 127, 4032 (**2023)**

84. N. Ahalawat, M. Sahil and **J. Mondal*** "Resolving Protein Conformational Plasticity and Substrate Binding via Machine Learning" *J. Chem. Theory Comput.* 19, 2644 (**2023)**

83. A Mondal, SN Save, S Sarkar, D Mondal, **J Mondal**, S Sharma, P Talukdar "A Benzohydrazide-Based Artificial Ion Channel that Modulates Chloride Ion Concentration in Cancer Cells and Induces Apoptosis by Disruption of Autophagy" *J. Am. Chem. Soc.* 145, 9737 (**2023)**

82. T. Maiti, P. Malik, S. Bawari, S. Ghosh, **J. Mondal** and R. Haldar "Chemically routed interpore molecular diffusion in metal-organic framework thin films" *Nature Comm.* 14, 2212 (**2023)**

81. N. Jamuna, A. Kamalakshan, B. Dandekar, A. Devassy, **J. Mondal**, and S. Mandal "Mechanistic Insight into the Amyloid Fibrillation Inhibition of Hen Egg White Lysozyme by Three Different Bile Acids" *J. Phys. Chem. B* in press, (**2023)**

80. M. Sahil, S. Sarkar and **J Mondal*** "Long-time-step molecular dynamics can retard simulation of protein-ligand recognition process" *Biophys. J.* 122, 802 (**2023)** (Featured as cover article)

79. S. Bawari, T. N. Narayanan and **J. Mondal*** "Insights into the reaction pathways of platinum dissolution and oxidation during electrochemical processes" *Electrochem. Comm.* 147, 107440 (**2023)**

78. A Wasim, A Gupta, P Bera, **J Mondal*** "Interpretation of organizational role of proteins on E. coli nucleoid via Hi-C integrated model" *Biophys. J.* 122, 63 (**2023)**

77. S. Bawari, A. Guha, T. N. Narayanan and **J. Mondal*** "Understanding Water Structure and Hydrogen Association on Platinum-Electrolyte Interface" *Oxford Open Mat. Sci.* 2, itac014 (**2023)**

76. A. Mondal, G. K. Barik, S. Sarkar, D. Mondal, M. Ahmad, T. Vijayakanth, **J. Mondal**, M. K. Santra and P. Talukdar "Nontoxic Artificial Chloride Channel Formation in Epithelial Cells by Isophthalic Acid-Based Small Molecules" *Chem. Euro. J.* 29, e202202887 (**2022)**

75. R. Dolai, R. Kumar, B. Elvers, P. Pal, B. Joseph,R. Sikari, M. Nayak, A. Maiti, T. Singh, N. Chryochos, A. Jayaraman, I. Krummernacher, **J. Mondal***, U. Deva Priyakumar, H. Braunschweig, C. B. Yilidiz, C. Schulzke, A. Jana "Carbodicarbenes and Striking Redox Transitions of their Conjugate Acids: Influence of NHC versus CAAC as Donor Substituents" *Chem. Euro. J.* 29, e202202888 (**2022)**

74. J. Singh, M. Sahil, S. Ray, C. Dcosta, S. Panjikar,G. Krishnamoorthy, **J. Mondal*** and R. Anand "Phenol sensing in nature modulated via a conformational switch governed by dynamic allostery" *J. Biol. Chem.* 298, 102399 (**2022)**

73. C. Mahato, S. Menon, A. Singh, S. Afrose, **J. Mondal** and D. Das "Short Peptide-based Cross- Amyloids Exploit Dual Residues for Phosphoesterase like Activity" *Chem. Sci.* 13, 9225 (**2022)**

72. D. Mondal, B. Dandekar, M. Ahmed, A. Mondal, **J. Mondal*** and P. Talukdar "Selective and Rapid Water Translocation across Self-assembled Peptide-Diol Channel via the Formation of Dual Water Array" *Chem. Sci.* 13, 9614 (**2022)**

71. S. Pal, J. Koneru, C. Andreou, T. Rakhsit, V. K. Rajsekhar, M. Wlodaryczyk, J. Healy, M. F. Kircher and **J. Mondal** "DNA-Functionalized Gold Nanorods for Perioperative Optical

Imaging and Photothermal Therapy of Triple-Negative Breast Cancer" *ACS Appl.Nano Mater.* 9, 9159 (**2022**)

70. S. Sarkar, A. Guha, T. N. Narayanan and **J Mondal*** "Zwitterionic Osmolytes Revive Surface Charges under Salt Stress via Dual Mechanisms" *J. Phys. Chem. Lett.* 13,5660 (**2022**)

69. B. B. Majumdar and **J Mondal*** "Impact of Inert Crowders on Host?Guest Recognition Process" *J. Phys. Chem. B* 126,4200 (**2022**)

68. P. Bera, A. Wasim and **J Mondal*** "Hi-C embedded polymer model of Escherichia coli reveals the origin of heterogeneous subdiffusion in chromosomal loci" *Phys. Rev. E* 105,064402 (**2022**)

67. S. Bandyopadhyay, B. B. Majumdar and **J Mondal*** "Solvent's Role in Cavity-Ligand Recognition Would Depend on the Mode of Ligand Diffusion" *J. Phys. Chem. B* DOI:10.1021/acs.jpcb.1c09645,in press (**2022**)

66. N. Sharma, S. Singh, A. S. Tanwar, **J. Mondal** and R. Anand "Mechanism of Coordinated Gating and Signal Transduction in Purine Biosynthetic Enzyme Formylglycinamidine Synthetase" *ACS Catalysis.* 12,1930 (**2022**)

65. J. Koneru, S. Sinha , **J Mondal*** "Molecular Dynamics Simulations Elucidate Oligosaccharide Recognition Pathways by Galectin-3 at Atomic Resolution" *J. Biol. Chem.* 297,101271 (**2021**)

64. B. Dandekar, S. Sinha , **J Mondal*** "Role of molecular dynamics in optimising ligand discovery: Case study with novel inhibitor search for peptidyl t-RNA hydrolase" *Chem. Phys. Impact* 3,1 (**2021**)

63. S. Bandyopadhyay and **J Mondal*** "A deep autoencoder framework for discovery of metastable ensembles in biomacromolecules" *J. Chem. Phys.* 155,114106 (**2021**)

62. S. Bawari, M. Nair, **J Mondal*** and T. N. Narayanan "Elucidating the Mechanism of Nitrogen Doping in Graphene Oxide: Structural Evolution of Dopants and the Role of Oxygen" *J. Phys. Chem. C* 125,22547 (**2021**)

61. J. Koneru, D. Prakashchand, N. Dube, P. Ghosh and **J Mondal*** "Spontaneous transmembrane pore formation by short-chain synthetic peptide" *Biophys. J.* 120,4557 (**2021**)

60. P. Bera, A. Wasim, **J Mondal** and P. Ghosh "Mechanistic underpinning of cell aspect ratio-dependent emergent collective motions in swarming bacteria" *Soft Matter* 17,7322 (**2021**)

59. S. Sarkar and **J Mondal*** "Mechanistic Insights on ATP's Role as a Hydrotrope" *J. Phys. Chem. B* 125,7717 (**2021**)

58. D. Prakashchand and **J Mondal*** "Conformational Reorganization of Apolipoprotein E Triggered by Phospholipid Assembly" *J. Phys. Chem. B* 125,5285 (**2021**)

57. B. Dandekar, N. Ahalawat and **J Mondal*** "Reconciling conformational heterogeneity and substrate recognition in cytochrome P450" *Biophys. J.* 120,1732 (**2021**)

56. A. Wasim, A. Gupta and **J Mondal*** "A Hi-C data-integrated model elucidates E. coli chromosome's multiscale organization at various replication stages" *Nucleic Acids Res.* 49,3077 (**2021**)

A2. As Reader (July 2015-June 2021)

55. A. Som, M. Pahwa, S. Bawari, N. Das Saha, R. Sasmal, M. S. Bosco, **J. Mondal** and S. S. Agasti "Multiplexed optical barcoding of cells via photochemical programming of bioorthogonal host-guest recognition *Chem. Sci.* 12,5484 (**2021**)

54. N. Ahalawat and **J. Mondal*** "An Appraisal of Computer Simulation Approaches in Elucidating Biomolecular Recognition Pathways *J. Phys. Chem. Letters* 12,633 (**2021**)

53. M. Mukherjee and **J. Mondal*** "Bottom-Up View of the Mechanism of Action of Protein-Stabilizing Osmolytes" *J. Phys. Chem. B* 124,11316 (**2020**)

52. M. Mukherjee and **J. Mondal*** "Unifying the Contrasting Mechanisms of Protein-Stabilising Osmolytes" *J. Phys. Chem. B* 124,6565 (**2020**)

51. B. R. Dandekar and **J. Mondal*** "Capturing Protein-Ligand Recognition Pathways in Coarse-grained Simulation" *J. Phys. Chem. Letters* 11,5302 (**2020**)

50. S Bawari, K Sharma, P Kalita, P K Madhu, TN Narayanan* and **J. Mondal*** "Engineering the hydrogen evolution reaction of transition metals: effect of Li ions" *Mater. Chem. Frontiers* 4,2330 (**2020**)

49. N Sharma, N Ahalawat, P Sandhu, E Strauss, **J Mondal**, R Anand "Role of allosteric switches and adaptor domains in long-distance cross-talk and transient tunnel formation" *Sci. Advances* 6,eaay7919 (**2020**)

48. P. D. Dheeraj, N. Ahalawat, S. Bandyopadhyay, S. Sengupta and **J. Mondal*** "Nonaffine Displacements Encode Collective Conformational Fluctuations in Proteins" *J.Chem. Theory Comput.* 16,2508 (**2020**)

47. N Ahalawat, S Bandyopadhyay and **J. Mondal*** "On the role of solvent in hydrophobic cavityligand recognition kinetics" *J.Chem. Phys.* 152,074104 (**2020**)

46. A Guha, S Narayanaru, NM Kaley, DK Rao, **J Mondal**, TN Narayanan "Engineering the hydrogen evolution reaction of transition metals: effect of Li ions" *J. Mater. Chem. A* 8,15795 (**2020**)

45. A Guha, S Narayanaru, NM Kaley, DK Rao, **J Mondal**, TN Narayanan "Mechanistic insight into high yield electrochemical nitrogen reduction to ammonia using lithium ions" *Materials Today Communications* 21100700(**2019**)

44. J. K. Koneru, X. Zhu and **J. Mondal*** "A Quantitative Assessment of the Conformational Heterogeneity in Amylose across Force Fields" *J.Chem. Theory Comput.* 15,6203 (**2019**)

43. M. Mukherjee and **J. Mondal*** "Osmolyte-Induced Macromolecular Aggregation is Length-scale Dependent" *J.Phys.Chem. B.* 123,8697 (**2019**)

42. J. K. Koneru and **J. Mondal*** "Quantitative Assessment of Amylose Dimerization Process across Force fields" *J.Indian Chem. Soc.*96,949 (**2019**) (Invited article on special issue)

41. B. Sarkar, Z. Siddiqui, P. K. Nguyen, N. Dube, W. Fu, S. Park, S. Jaisinghani, R. Paul, S. D. Kozuch, D. Deng, P. Montoro,M. Li, D. Sabatino,D. S. Perlin,W. Zhang, **J. Mondal** and V. A. Kumar "Membrane-Disrupting Nanofibrous Peptide Hydrogels" *ACS Biomater. Sci. Eng* 5,4657 (**2019)**

40. J. K. Koneru, S. Sinha and **J. Mondal*** "In Silico Re-Optimization of Binding Affinity and Drug-Resistance Circumvention Ability in Kinase Inhibitors:Case study with RL-45 and Src kinase" *J.Phys.Chem. B*123,6664 (**2019)**

39. S. Bawari, S. Pal, S. Pal, **J. Mondal*** and T. N. Narayanan "Enhanced Photo-Electrocatalytic Hydrogen Generation in Graphene/hBN van der Waals Structure" *J.Phys.Chem. C* 123,17249 (**2019)**

38. M. Mukherjee and **J. Mondal*** "Osmolyte-Induced Collapse of a Charged Macromolecule" *J.Phys.Chem. B.* 123,4636 (**2019)**

37. S. Pal, A. Ray, C. Andreou, Y. Zhou, T. Rakshit, M. Wlodarczyk, M. Maeda, R. Toledo-Crow, N. Berisha, J. Yang, H. Hsu, A. Oseledchyk, **J. Mondal**, S. Zou and M. F. Kircher "DNA-enabled rational design of fluorescence-Raman bimodal nanoprobes for cancer imaging and therapy" *Nature Communications* 10, 1926 (**2019)**

36. M. Mukherjee and **J. Mondal** and S. Karmakar "Role of α and β relaxations in collapsing dynamics of a polymer chain in supercooled glass-forming liquid" *J.Phys.Chem. B.* 150, 114503 (**2019)**

35. **J. Mondal*** "A brief appraisal of computational modeling of antimicrobial peptides activity" *Drug Development Research* 80, 28 (**2019)**

34. D. Dube, N. Ahalawat, H. Khandelia, **J. Mondal*** and Surajit Sengupta* "On identifying collective displacements in apo-proteins that reveal eventual binding pathways" *PLOS Comput. Biol.* 15, e1006665 (**2019)**

33. N. Ahalawat and **J. Mondal*** "Mapping the Substrate Recognition in Cytochrome P450" *J.Am.Chem.Soc.* 140, 17743 (**2018)**

32. N. Ahalawat and **J. Mondal*** "Assessment and optimization of collective variables for protein conformational landscape: GB1 β-hairpin as a case study" *J.Chem.Phys.* 149, 094101 (**2018)** (Feature Article and cover)

31. M. Mukherjee and **J. Mondal*** "Heterogeneous Impacts of Protein-Stabilizing Osmolytes on Hydrophobic Interaction" *J.Phys.Chem.B.* 122, 6922 (**2018**

30. **J. Mondal***,N. Ahalawat, S. Pandit, L. Kay and P. Vallurupalli "Atomic resolution mechanism of ligand binding to a solvent inaccessible cavity in T4 lysozyme" *PLOS Comput. Biol.* 14, e1006180 (**2018)**

29. S Bawari,T N. Narayanan and **J Mondal*** "Atomistic Elucidation of Sorption Processes in Hydrogen Evolution Reaction on a van der Waals Heterostructure" *J. Phys. Chem. C* 122, 10034 (**2018)**

28. S Bawari,N. M. Kaley, S. Pal, T. V. Vineesh, S. Ghosh, T. N. Narayanan and **J Mondal*** "On the hydrogen evolution reaction activity of graphene-hBN van der Waals heterostructures" *Phys. Chem. Chem. Phys.* 20, 15007 (**2018)**

27. Y Lyu, N Xiang, **J Mondal**, X Zhu and G Narsimhan "Characterization of Interactions between Curcumin and Different Types of Lipid Bilayers by Molecular Dynamics Simulation" *J. Phys. Chem. B* 122, 2341 (**2018)**

26. A. Ray, N. Ahalawat and **J. Mondal*** "Atomistic Insights into Structural Differences between E3 and E4 Isoforms of Apolipoprotein E" *Biophys. J.* 113, 2682 (**2017)**

25. S Ray, A Maitra, A Biswas, S Panjikar, **J Mondal**, R Anand "Functional Insights into the Mode of DNA and Ligand Binding of the TetR Family Regulator TylP from Streptomyces fradiae" *J. Biol. Chem.* 292, 15301 (**2017)**

24. P. Tiwary,**J. Mondal** and B. J. Berne "How and when does an anticancer drug leave its binding site?" *Science Advances* 3, e1700014 (**2017)**

23. R. Berkovich, **J. Mondal***, I. Paster and B. J. Berne "Simulated Force quench Dynamics shows GB1 protein is not a two-state folder" *J. Phys. Chem. B* 121, 5162 (**2016)**

22. I. Tah and **J. Mondal*** "How does a hydrophobic macromolecule respond to a mixed osmolyte environment?" *J. Phys. Chem. B* 120, 10969 (**2016)**

21. **J. Mondal***, P. Tiwary and B. J. Berne "How does kinase inhibitor withstand gate-keeper residue mutation" *J. Am. Chem. Soc.*138, 4608 (**2016)**

B. During doctoral and Postdoctoral tenure (2007- June 2015)

20. S. Roy, D. Skoff, D. Perroni, **J. Mondal**, A. Yethiraj, M. K. Mahanthappa, M. T. Zanni and J. L. Skinner "Water Dynamics in Gyroid phases of self-assembled gemini surfactants" *J. Am. Chem. Soc.* 138,2472 (**2016)**

19. P. Tiwary, **J. Mondal**, J. A. Morrone and B. J. Berne "Role of water and steric constraints in the kinetics of cavity-ligand unbinding" *Proc. Natl. Acad. Sci. USA* 112,12015 (**2015)**

18. **J. Mondal**, D. Halverson, I.T.S. Li, G. Stirnemann, G. C. Walker and B. J. Berne "How osmolytes influence hydrophobic polymer conformations: A unified view from experiment and theory" *Proc. Natl. Acad. Sci. USA* 112,9270 (**2015)**

17. P. Ghosh, **J. Mondal**, E. Ben-Jacob and H. Levine "Mechanically-driven depletion-mediated pattern formation in a growing bacterial colony" *Proc. Natl. Acad. Sci. USA* 112, E2166 (**2015)**

16 . **J. Mondal**, R. A. Friesner and B. J. Berne, "Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase" *J.Chem. Theory Comput.* 10, 5696(**2014)**

15. . S. Bakshi, H. Choi, **J. Mondal** and J. C. Weisshaar, "Time-dependent Effects of Transcription- and Translation-halting Drugs on the Morphology of the Escherichia coli" *Mol. Micro.* 94, 871 (**2014)**

14. **J. Mondal**, E. Choi and A. Yethiraj, "Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature" *Macromolecules* 47, 438 (**2014)**

13. E. Choi, **J. Mondal** and A. Yethiraj, "Coarse-grained models for aqueous polyethylene glycol solutions" *J. Phys. Chem. B* 118, 323 (**2014)**

12. **J. Mondal**, J. A. Morrone and B. J. Berne, "How hydrophobic drying forces impact the kinetics of molecular recognition " *Proc. Natl. Acad. Sci. USA* 110, 13277 (**2013)**

11. **J. Mondal**, G. Stirnemann and B. J. Berne, "When does Trimethyl N-oxide fold a polymer chain and urea unfold it?", *J.Phys.Chem. B* 117, 8723 (**2013)**

10. **J. Mondal**, M. Mahanthappa and A. Yethiraj, "Self-assembly of Gemini surfactants:A computer simulation study", *J. Phys. Chem. B* 117, 4254 (**2013).**

9. **J. Mondal** and A. Yethiraj, "Effect of secondary structure on self-assembly of amphiphilic molecules", *J. Chem. Phys.* 136, 084902 (**2012).**

8. **J. Mondal**, X. Zhu, Q. Cui and A. Yethiraj, "Insights on sequence-dependent pKa-shift in catalytic reactions of β-peptide foldamers: Computer-simulation study", *J. Phys. Chem. B* 116, 491 (**2012).**

7. **J. Mondal** and A. Yethiraj, "The driving force for the association of amphiphilic molecules", *J. Phys. Chem. Lett.* 2, 2391 (**2011).**

6. **J. Mondal**, B. P. Bratton, Y. Li, A. Yethiraj and J. C. Weisshaar, "Entropy-based mechanism of ribosome-nucleoid segregation in E.coli cells", *Biophys. J.* 100, 2605 (**2011).**

5. **J. Mondal**, X. Zhu, Q. Cui and A. Yethiraj, "Sequence-dependent interaction of β-peptides with membranes", *J. Phys. Chem. B* 114, 13585 (**2010).**

4. **J. Mondal**, X. Zhu, Q. Cui and A. Yethiraj, "Self-assembly of β-peptides: Insights from pair and many-body free energy of association", *J. Phys. Chem. C* 114, 13551 (**2010).**

3. **J. Mondal**, B. J. Sung and A. Yethiraj, "Sequence-dependent self-assembly of β-peptides : Insights from coarse-grained model", *J. Chem. Phys* 132, 065103 (**2010).**

2. **J. Mondal**, B. J. Sung and A. Yethiraj, "Sequence-dependent organization of β-peptides in self-assembled monolayers", *J. Phys. Chem. B* 113, 9379 (**2009).**

1. V. Sharma, B. Bapat, **J. Mondal**, M. Hochlaf, K. Giri and N. Sathyamurthy, "Dissociative double ionization of CO_2 : Dynamics, energy levels and lifetimes", *J. Phys. Chem. A* 111, 10205 (**2007).**

Funded research projects:

1. Jagannath Mondal, Xiao Zhu *'Mechanistic Investigation anti microbial peptides in action using large-scale computer simulations*',
Extreme Science and Engineering Discovery Environment (XSEDE), USA for Computational allocation (allocation provided in San diego Supercomputer), 1 year (September 2018-June 2019)

2. Jagannath Mondal '*Elucidation of kinetic pathways of protein-ligand recognition and improvement of virtual drug discovery using Computer simulation*'
Early Career Research, DST-SERB (INR 52 Lakhs) (September 2016- September 2019)

3. Jagannath Mondal '*Inference of long-time biochemical processes via combination of short-length Molecular Dynamics simulation with Markov State Model*'
Core Research grant, DST-SERB (INR 47 Lakhs) (January 2020-December 2023)

Conference Organizations:

1. Co-organized *RARE2020* an international conference in Rare-event sampling (2021 Online, due to Covid)
2. Organized *Molecular Simulation: Focus on Method* to gain tractions on developmental researches in Molecular simulation (TIFR Hyderabad, December 2022)
3. Co-organizer of monthly online *Integrative Modelling Webinar Series* for international community (Online, 2022-present)
4. Co-organized *ML4Science 2023* to foster interest in Machine-learning based research in Indian scientific community (March, 2023, Kodaikanal, Tamil Nadu)

Graduate Courses taught at TIFR-H

1. Statistical Mechanics I (5 semesters)
2. Numerical Methods and Algorithms in Chemical Physics (2 semester)
3. Molecular and Nonlinear Dynamics (2 semesters)
4. Molecular Dynamics Simulation (2 semester)
5. Polymer Physics (1 semester)