Curriculum-Vitae

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

Full Correspondence Address

Tata Institute of Fundamental Research
Hyderabad
36/P Gopanapalli village, Serilingampalli mandal,
PIN- 500046

E-mail : jagannath.mondal@gmail.com
jmondal@tifrh.res.in
Phone : 8978800599
Webpage: https://www.tifrh.res.in/ jmondal/

Work experience (In Chronological order)

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

Academic Qualification (Undergraduate Onwards)

- Ph. D. at University of Wisconsin Madison, USA (Advisor: Arun Yethiraj) 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

- Young Associate of Indian Academy of Scicences 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 (Bio)molecular recognition processes and Drug Discovery
- Molecular Dynamics simulation of protein folding and interaction of osmolytes
- Understanding Biological membrane and its interaction with protein
- Understanding sub-cellular organization of bacterial and eukaryotic cytoplasm
- Modelling Materials science and hydrogen evolution reaction

Brief Research Accomplishments

1. Atomistic Mechanism of protein-ligand recognition and elucidation of kinetic pathways of ligand binding/unbinding process in multiple biochemical systems via unbiased Molecular Dynamics simulation and Markov state model at an atomistic precision and in real time. (Dandekar et al *J.Phys.Chem. Letters (2020)*, Mondal et al *PLOS Comput. Biol. (2018)* , Ahalawat et al *J. Am. Chem. Soc.(2018)* and Tiwary et al *Science Advances (2017)*).

2. Deciphering the mechanism of drug resistance via Molecular Dynamics simulations and computational discovery of potential drug molecules. (Mondal et al *J.Am.Chem.Soc.(2016)* and Koneru et al *J.Phys.Chem. B(2019)*)

3. Assessment and optimization of key collective variables for quantifying key biophysical processes namely protein-folding and protein-ligand binding (Berkovich et al *J.Phys.Chem. B(2017)*, Ahalawat et al *J.Chem.Phys.(2018)* and Prakashchand et al *PLOS Comput. Biol. (2019)*)

4. Dissection of mechanistic role of osmolyte on hydrophobic interactions via computer simulations. (Tah et al *J.Phys.Chem. B (2016)*, Mukherjee et al *J.Phys.Chem. B (2018)*, Mukherjee et al *J.Phys.Chem. B (2019)*)

5. Providing a physical picture of cellular and sub-cellular organization of bacteria. (Wasim et al *Nucleic Acids Res.(2021)*, Bera et al *Soft Matter(2021)*)

6. Rendering computational support and collaborations to experimentalists within India and outside India in the field of physical, biochemical and material sciences . (Sharma et al*Sci. Advances (2020)*, Sarkar et al *ACS Biomater. Sci. Eng. (2019)*, Bawari et al *J.Phys.Chem. C (2018)*, Bawari et al *Phys.Chem.Chem.Phys.(2018)*, Pal et al *Nature Comm.(2019)*,Lyu et al *J.Phys.Chem. B(2018)*, Ray et al *J.Biol.Chem.(2017)*)

Publications

As a Principal Investigator (July 2015-present)

(* : As Corresponding author)

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* in press,doi:10.1039/D1SM00311A (**2021)**

59. S. Sarkar and **J Mondal*** "Mechanistic Insights on ATPs 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. Dadekar, N. Ahalawat and **J Mondal*** "A HiC data-integrated model elucidates E. coli chromosomes multiscale organization at various replication stages *Biophys. J.* 120,1732 (**2021**)

56. A. Wasim, A. Gupta and **J Mondal*** "A HiC data-integrated model elucidates E. coli chromosomes multiscale organization at various replication stages *Nucleic Acids Res.* 49,3077 (**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 hostguest 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)**

During doctoral and Postdoctoral tenure (Till 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)

Student Guidance

1. PhD students: 10 (1 received PhD, 2 would defend thesis in August)
2. Postdoctoral associate: 5 (3 completed terms and joined faculty/postdoc abroad)

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)