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| **Arnab Mukherjee**  **Associate Professor**  **Department of Chemistry**  **Indian Institute of Science Education and Research, Pune**  **Telephone: +92 2590 8051**  **Email: arnab.Mukherjee@iiserpune.ac.in,** [**dr.arnab.mukherjee@gmail.com**](mailto:dr.arnab.mukherjee@gmail.com)  **Date of Birth: August 8, 1977** | | | | | | | | |
| Education | | | | | | | | |
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| B. Sc. In Chemistry | | July 1998 | | | | | |
| Jadavpur University, Kolkata, West Bengal, India  Honors: 1st Class | | | | | | | |
|  | | | | | | | |
| M.S. in Chemical Sciences (Integrated Ph.D. Program) | | July 2001 | | | | | |
| Chemical Sciences, Indian Institute of Science, Bangalore, India  M.S. Thesis: “Transport properties in binary mixture”  Advisor: Prof. Biman Bagchi  Honors: 1st class | | | | | | | |
|  | | | | | | | |
| Ph. D. in Theoretical/Computational Chemistry | | May 2005 | | | | | |
| Solid state and Structural Chemistry Unit,  Indian Institute of Science, Bangalore, India  Dissertation: “From Transport Properties of Binary Mixture to Dynamics of Protein Folding and Some Contributions to the Rotational Friction of Proteins”  Advisor: Prof. Biman Bagchi  Honors: Best Thesis Award and Sudborough Medal | | | | | | | |
| Professional Experience | | | | | | | | |
|  | | Indo-French Postdoctoral Fellowship,  Ecole Normale Superieure, Paris, France  Advisor: Prof. James T. Hynes  Topic: Mechanism of intercalation of anticancer drugs into DNA  Department of Chemistry and Biochemistry,  University of Colorado, Boulder  Advisor: Prof. James T. Hynes  Topic: Mechanism of peptide bond formation in ribosome  Assistant Professor  Department of Chemistry,  Indian Institute of Science Education and Research, Pune, India  Associate Professor  Department of Chemistry,  Indian Institute of Science Education and Research, Pune, India | | | June 2005 -  May 2007 | | | |
| June 2007 -  October 2009  **November 2009 -**  **November 2015**  **November 2015 -**  **Present** | | | |
| Research TOPICS | | | | | | | | |
|  | | 1. **Mechanism of drug intercalation into DNA** 2. **Entropy of water molecules and their role in protein-ligand binding** 3. **Protein-DNA interaction** 4. **Understanding the mechanism of enzyme mediated reaction processes in biological systems** 5. **Dynamics of water around biomolecules** 6. **Structure/Dynamics of DNA** 7. **Dynamical Recrossing** 8. **Protein Folding/Misfolding** 9. **Machine learning and deeplearning based drug design** | | | |  | |
| Publications | | | | | | | | |
|  | | 1. “Nonideality in Publications the Composition Dependence of Viscosity in Binary Mixtures”, Goundla Srinivas, **Arnab Mukherjee** and Biman Bagchi, J. Chem. Phys. 114, 6220 (2001).  2. “Reentrant Behavior of Relaxation Time with Viscosity at Varying Composition in Binary  Mixtures”, **Arnab Mukherjee**, Goundla Srinivas and Biman Bagchi, Phys. Rev. Lett. 86,  5926 (2001).  3. “Nonideality in Binary Mixture: Correlation between Excess volume, Excess Viscosity  and Diffusion Coefficients”, **Arnab Mukherjee** and Biman Bagchi, J. Phys Chem. B 105,  9581 (2001).  4. “Ionic Self-Diffusion in Concentrated Electrolyte Aqueous Solutions”, J.-F. Dufreche, O.  Bernard and P. Turq, **Arnab Mukherjee** and Biman Bagchi, Phys. Rev. Lett. 88, 95902  (2002).  5. “Pressure and Temperature Dependence of Viscosity and Diffusion Coefficients in Glassy  Binary Mixture”, **Arnab Mukherjee**, Sarika Bhattacharyya and Biman Bagchi, J. Chem.  Phys. 116, 4577 (2002).  6. “Correlated orientational and translational motions in supercooled liquids”, Sarika Bhattacharyya, **Arnab Mukherjee** and Biman Bagchi, J. Chem. Phys. 117, 2741 (2002).  7. “Relaxation in binary mixtures: Non-ideality, heterogeneity and re-entrance”, **Arnab**  **Mukherjee**, Goundla Srinivas, Sarika Bhattacharyya and Biman Bagchi, Proc. Ind. Acad.  Sci. (Chem. Sci.), 113, 393 (2001).  8. “Correlation between rate of folding, topology and energy landscape of a model protein  HP-36”, **Arnab Mukherjee** and Biman Bagchi, J. Chem. Phys. 118, 4733 (2003).  9. “Origin of the sub-diffusivity behavior and crossover from sub-diffusive to super-diffusive dynamics near biological surface”, **Arnab Mukherjee** and Biman Bagchi, Phys. Chem.  Comm. 6, 28 (2003).  10. “Fluorescence resonance energy transfer dynamics during protein folding: Evidence of  multistage folding kinetics”, **Arnab Mukherjee** and Biman Bagchi, Curr. Sci., 85, 68 (2003).  11. “Probing folding free energy landscape of small proteins through minimalistic models:  Folding of HP-36 and beta -amyloid”, **Arnab Mukherjee** and Biman Bagchi, Proc. Indian  Acad. Sci. (Chem. Sci.), 115, 620 (2003).  12. “Contact pair dynamics during folding of two small proteins: Chicken villin head piece  and the Alzheimer protein beta-amyloid”, **Arnab Mukherjee** and Biman Bagchi, J. Chem.  Phys., 120, 1602 (2004).  13. “Rotational friction on globular proteins combining dielectric and hydrodynamic effects”  **Arnab Mukherjee** and Biman Bagchi, Chem. Phys. Lett., 404, 409 (2005).  14. “Orientation-dependent potential of mean force for protein folding” **Arnab Mukherjee**, Prabhakar Bhimalapuram, and Biman Bagchi, J. Chem. Phys. 123, 014901 (2005).  15. “Fröster energy transfer in thin films of conjugated polymers and in solution, **A. Mukherjee**  and B. Bagchi, J. Chin. Chem. Soc.” 53, 153 (2006).  16. “Anomalous orientation dependent effective pair interaction among histidine and other  amino acid residues in metalloproteins: Breakdown of the hydropathy scale index” **Arnab**  **Mukherjee** and Biman Bagchi, Biochemistry, 45, 5129 (2006).  17. "Solvent Frictional Forces in the rotational diffusion of proteins in water", **Arnab Mukherjee** and Biman Bagchi, Curr. Sci. 91, 1208 (2006).  18. “On the molecular mechanism of drug intercalation into DNA: A computer simulation study of the intercalation pathway, free energy and DNA structural changes”, **Arnab Mukherjee\***, Richard Lavery, Biman Bagchi and James T. Hynes, J. Am. Chem. Soc. 130, 9747 (2008).  19. *(invited Book Chapter):* Simulation Study of Free Energy and Molecular Mechanism of Intercalation of the Anti-Cancer Drug Daunomycin into DNA, **A. Mukherjee**, R. Lavery, B. Bagchi, and James T. Hynes, in "Energy Transfer Dynamics in Biomaterial Systems", Eds. I. Burghardt, V. May, D. A. Micha, and E. R. Bittner, Springer Series in Chemical Physics, Vol. 93, 2009). | | | | | | |
| Publications From iiser, Pune | | | |
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| 20. “Entropy Balance in the Intercalation Process of an Anti-Cancer Drug Daunomycin” **Arnab Mukherjee\***, J. Phys. Chem. Lett. 2, 3021 (2011).  21. “Comparative Study of flavins’ binding with human serum albumin: a fluorometric, thermodynamic, and molecular dynamics approach“, Abhigyan Sengupta, D. S. Wilbee, **Arnab Mukherjee\***, Partha Hazra\* *(Submitted to Chem. Phys. Chem.)*  22. “A multistep intercalation mechanism: molecular dynamics and free energy studies of the formation of a DNA-daunomycin complex”, M. Wilhelm, **A. Mukherjee\***, B. Bouvier, K. Zakrzewska, J.T. Hynes\*, R. Lavery\* J. Am. Chem. Soc. 134, 8588 (2012). (Received JACS spotlight: "A Computational Approach to Interpreting Intercalation" by E. J. Gordon. Link http://pubs.acs.org/doi/full/10.1021/ja305429h)  23. “Molecular Mechanism of Direct Proflavine-DNA Intercalation: Evidence for Drug-Induced Minimum Base-Stacking Penalty Pathway”, Wilbee D. S. and **A. Mukherjee\*** J. Phys. Chem. B 116, 12208 (2012).  24. “Modulation of Excimer Formation of 9-(dicyano-vinyl)julolidine by the Macrocyclic Hosts”, Krishna Gavvala, Wilbee D Sasikala, Abhigyan Sengupta, Siddhi A Dalvi, **Arnab Mukherjee** , and Partha Hazra\*, Phys. Chem. Chem. Phys., **15**, 330 (2013).  25. “Intercalation and De-intercalation Pathway of Proflavine through the Minor and Major Grooves of DNA: Role of Water and Entropy”, Wilbee D Sasikala and **Arnab Mukherjee\*** , Phys. Chem. Chem. Phys., **15**, 6446 (2013).  26. *(invited book chapter)* “ Drug-DNA Intercalation: From Discovery to the Molecular Mechanism ”, **Arnab Mukherjee\*** and Wilbee D. Sasikala in Dynamics of Proteins and Nucleci Acids, Vol. 92, Series: Advances in Protein Chemistry and Structure Biology, Ed. Tatyana Karabencheva, UK: Academic Press, 2013, pp. 1-62.  27. “Sequence Dependent Free Energy Profiles of Localized B- to A-Form Transition of DNA in Water”, Mandar Kulkarni and **Arnab Mukherjee\*** J. Chem. Phys. 139, 155102 (2013).  28. “Urea Induced Unfolding Dynamics of Flavin Adenine Dinucleotide (FAD): Spectroscopic and Molecular Dynamics Simulation Studies from Femto-Second to Nanosecond Regime”, A. Sengupta, Reman K. Singh, Krishna Gavvala, Raj Kumar Koninti, **Arnab Mukherjee\***, and Partha Hazra\*. J. Phys. Chem. B 2014 (in press).  29. “Single Water Entropy: Hydrophobic Crossover and Application to Drug Binding”, Wilbee D. Sasikala and **Arnab Mukherjee\***J. Phys. Chem. B 118, 10553 (2014).  30. “Hopping Mediated Anion Transport through a Mannitol-Based Rosette Ion Channel”, Tanmoy Saha , Sathish Dasari , Debanjan Tewari , Annamalai Prathap , Kana M. Sureshan , Amal K. Bera\*, **Arnab Mukherjee\***, and Pinaki Talukdar\* J. Am. Chem. Soc. 136, 14128 (2014).  31. “Theoretical Study of Structural Changes in DNA under High External Hydrostatic Pressure”, P. Sudheer Kumar, **Arnab Mukherjee\***, and Anirban Hazra\* J. Phys. Chem. B 119, 3348 (2015).  32. “Distribution of Residence time of water around DNA Base Pairs: Governing Factors and the Origin of Heterogeneity”, Debasis Saha, Shreyas Supekar, and **Arnab Mukherjee\***J. Phys. Chem. B 119, 11371 (2015). *Biman Bagchi Festschrift*  33. “Molecular Origin of DNA Kinking by Transcription Factors”, Reman K. Singh, Wilbee D. Sasikala, and **Arnab Mukherjee\***, J. Phys. Chem. B 119, 11590 (2015).  34. “Computational Approach to Explore B/A Junction Free Energy in DNA” Mandar Kulkarni and **Arnab Mukherjee\***, Chem. Phys. Chem. (in press: DOI: 10.1002/cphc.201500690).  35. “Structure and Dynamics of Proflavine Association around DNA", Wilbee D. Sasikala and **Arnab Mukherjee\***, Phys. Chem. Chem. Phys. 18, 10383 (2016).  36. “Ionic Liquid Prolongs DNA Translocation through Graphene Nanopore", Mandar Kulkarni\* and **Arnab Mukherjee\***, RSC Advances . (in press).  37. "An Ultrahydrophobic Fluorous Metal-organic Framework Derived Recyclable Composite As A Promising Platform to Tackle Marine Oil Spills", Soumya Mukherjee, Ankit M. Kansara, Debasis Saha, Rajesh Gonnade, Dinesh Mullangi, Biplab Manna, Aamod V. Desai, **Arnab Mukherjee**, and Sujit K. Ghosh, Chemistry - A European Journal, 22, 10937 (2016).  38. "Impact of Ions on Invidial Water Entropy" Debasis Saha and **Arnab Mukherjee\***, J. Phys. Chem. B 120, 7471 (2016).  39. "Ionic Liquid Induced G-quadruplex Formation and Stablization: Spectroscopic and Simulation Studies" Sagar Satpati, Mandar Kulkarni, **Arnab Mukherjee\***, Partha Hazra\*, Phys. Chem. Chem. Phys. (in press).  40. "One-pot Synthesis and Transmembrane Chloride Transport Properties of C3-Symmetric Benzoxazine Urea" Arundhati Roy, Debasis Saha, **Arnab Mukherjee**, Pinaki Talukdar, Org. Lett. (in press).  41. "Water modulates the ultraslow dynamics of hydrated ionic liquids near CG rich DNA: consequence to DNA stability " Debasis Saha\*, Mandar Kulkarni, and **Arnab Mukherjee\***, Phys. Chem. Chem. Phys. 18, 32107 (2016).  42. "pH-Gated Chloride Transport by Triazine-based Tripodal Semicage", Arundhati Roy, Debasis Saha, Prashant Sahebrao Mandal, **Arnab Mukherjee**, and Pinaki Talukdar\*, Chemistry - A European Journal, 23 1241 (2017).  43. "Chloride Transport through Supramolecular Barrel-Rosette Ion Channels: Lipophilic Control and Apoptosis-Inducing Activity", Tanmoy Saha, Amitosh Gautam, **Arnab Mukherjee**, Mayurika Lahiri, Pinaki Talukdar\*, J. Am. Chem. Soc. 138, 16443 (2017).  44. "Mechanism of Unfolding of Human Prion Protein", Reman K. Singh, Neharika G. Chamachi, Suman Chakrabarty\*, and **Arnab Mukherjee\***, J. Phys. Chem. B 121, 550 (2017).  45. "Broadband Terahertz Dielectric Spectroscopy of Alcohols " Sohini Sarkar, Debasis Saha, Sneha Banerjee, **Arnab Mukherjee**, and Pankaj Mondal\*, Chem. Phys. Lett. 678 65 (2017).  46. “Connecting diffusion and entropy of bulk water at the single particle level”, Debasis Saha and **Arnab Mukherjee\*,** J. Chem. Sci. 129, 825 (2017).  47. “Understanding B-DNA to A-DNA transition in the right-handed DNA helix: Perspective from a local to global transition”, Mandar Kulkarni and **Arnab Mukherjee\***, 128, 63 (2017).  48. "Self-assembly of small-molecule fumaramides allows transmembrane chloride channel formation " Arundhati Roy, Amitosh Gautam, Javid Ahmad Malla, Sohini Sarkar, **Arnab Mukherjee**and Pinaki Talukdar, Chem. Comm. (doi: 10.1039/C7CC08693H)  49. "Effect of Water and Ionic Liquids on Biomolecules" Debasis Saha and **; Arnab Mukherjee\***;, Biophys. Rev. (in press).  50. " Controlling an Anticancer Drug Mediated G-quadruplex Formation and Stabilization by a Molecular Container” Sagar Satpathi, Reman K. Singh, **Arnab Mukherjee\*,** and Partha Hazra\*, Phys. Chem. Chem. Phys. (in press).  51. "Design of Bivalent Nucleic Acid Ligands for Recognition of RNA2 Repeated Expansion Associated with Huntington’s Disease" Shivaji A. Thadke, J. Dinithi R. Perera, V. M. Hridya, Kirti Bhatt,Ashif Y. Shaikh, Wei-Che Hsieh, Mengshen Chen, Chakicherla Gayathri, Roberto R. Gil, Gordon S. Rule, **Arnab Mukherjee**, Charles A. Thornton, and Danith H. Ly\*, Biochemistry, 57, 2094 (2018).    52. "Probing the Viscosity Dependence of Rate: Internal Friction or the Lack of Friction?" V. M. Hridya and **Arnab Mukherjee\***, J. Phys. Chem. B 122, 9081 (2018)    53. "Shape-Selective Bifacial Recognition of Double Helical B-DNA" Shivaji A. Thadke, J. Dinithi R. Perera, V. M. Hridya, Roberto R. Gil, **Arnab Mukherjee**, and Danith H. Ly\*, Communications Chem. (in press).  54. “Dynamical Recrossing in the Intercalation Process of the Anticancer Agent Proflavine into DNA”, V. M. Hridya and **Arnab Mukherjee\*,** J. Phys. Chem. B ([doi:10.1021/acs.jpcb.9b08470](https://pubs.acs.org/doi/10.1021/acs.jpcb.9b08470)).   * 55. “Arresting an Unusual Amide Tautomer Using Divalent Cations”, [Somnath M. Kashid](https://pubs.acs.org/action/doSearch?field1=Contrib&text1=Somnath%0AM.++Kashid), Reman K. Singh, Hyejin Kwon, Yung Sam Kim**\***, **Arnab Mukherjee\***, Sayan Bagchi**\*,** J. Phys. Chem. B, 123, 8419-8424 (2019). | | | | |

***\*corresponding author***

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| Invited and Contributed Talks | |
| 1. (***invited****)* Entropy Balance in the Intercalation Process of an Anti-Cancer Drug Daunomycin, NCL, Pune 2012. 2. (***invited***) “Molecular Mechanism of Intercalation”, delivered in a conference … I.I.I.T, Hyderabad, 2012. 3. (***Invited***) “Molecular Mechanism of Intercalation” delivered in the conference titled “Computer Assisted Drug Designing and Green Chemistry" organised by Department of Chemistry, Career College, Bhopal. (January 2013). 4. (***Contributed***) “Molecular Mechanism of Proflavine Intercalation: Evidence for Drug- Induced Minimum Base-stacking Penalty Pathway” delivered at the 57th Biophysical Society Conference, Philadelphia, USA (February 2013). 5. (***Invited***) “On the role of water entropy around biomolecules and in recognition processes” delivered at Glasgow University, UK under a collaborative effort funded by UKERIE. (June 2013). 6. (***Contributed***) “Molecular Mechanism of Proflavine Intercalation into DNA” delivered at Edinburg University, UK under a collaborative effort funded by UKERIE (June 2013). 7. (***invited****)* “Molecular Mechanism of Proflavine Intercalation into DNA” ICBSD IIT Chennai, November 28-30, 2013. 8. (***invited Poster****)* “Variation of single water entropy around hydrophobic, weakly attractive and charged solutes”, SM-YIM, Poindicherry, January 5-8, 2014. 9. (***invited****)* “Molecular Mechanism of Proflavine Intercalation into DNA”, IIT Kanpur, February 2014. 10. *(****invited****)* “On the structural transition of DNA at a local level.” IMSc Chennai, February 2014. 11. (***invited poster****)* “Single Water Entropy” at MD@50, JNCASR, Bangalore, August 2014. 12. (***invited*** ) “On the Mechanism of Intercalation.” ASUD, IACS, Kolkata, December 2014. 13. (***invited)***“Single Water Entropy: Hydrophobic Crossover and Application to Drug Binding”, Theoretical Chemistry Symposium(TCS), December 2014. 14. (***invited)*** *“Molecular Mechanism of Intercalation”, Workshop by Param Uva II, January 2015.* 15. (***invited)*** *“On the Mechanism of Intercalation”, ISBOC, IISER, Pune, January 10, 2015.* 16. (***invited)*** *“On the Molecular Mechanism of Intercalation”, In “Accelerating Biology2015: Catalyzing Evolution” January 20, 2015* 17. (***invited****)* “On the Molecular Mechanism of Proflavine Intercalation to DNA”, KTH Royal Institute of Technology, Sweden. (June 2015). 18. **(*Contributed*)** “Mechanism of DNA Intercalation of anti-cancer agent proflavine”, In the conference entitled “exploring mechanism in biology”, A\* University, Singapore. (November 2015). 19. (***invited****)* “Single Water Entropy: Hydrophobic Crossover and Application to Drug Binding”, In a symposium called “IISER Pune-Temple University joint symposium” (December 2015). 20. (***invited****)* “Distribution of Residence Time of Water around DNA: Origin of Heterogeneity” Inter IISER Chemistry Meet, Trivandrum (December 2015). 21. (***invited****)* “How does a ligand get intercalated into a double helical DNA?”, Bose Institute, Kolkata (January 2016). |

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| List of Project implemented |

16.1 Details of Projects in progress

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| S.No. | Title | Cost in Lakh | Duration | Role  (PI/Co-PI) | Agency |
| 1. | Teachers Associateship for Research Excellence (TARE) to Dr. Sunil Patil | 7,50,000 | 3 years | Mentor | SERB, DST, India |

16.2 Details of Projects completed

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| S.No. | Title | Cost in Lakh | Duration | Role  (PI/Co-PI) | Agency |
| 1. | Dynamical effects in the mechanism of intercalation of anti-cancer drugs | 50,00,000 | 20/05/2013-19/05/2016 | PI | SERB, DST, India |
| 2. | Connecting the Kinetics and Thermodynamics of Solvation Shell Water at the Local Level: Effect of Chemical and Topographical Heterogeneity | 48,91,700 | 19/09/2016-18/09/2019 | PI | SERB, DST, India |