Biographical sketch of Dr. S. Chowdhuri

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Educational Qualification:

Ph. D., Theoretical Chemistry, 2005, Indian Institute of Technology Kanpur, India.
M. Sc., Physical Chemistry, 1996, The University of Burdwan, West Bengal, India.
B. Sc., (Chemistry *honours*), 1994, The University of Burdwan, West Bengal, India.

Research Experience:

1998-2004 Pre doctoral Research, Indian Institute of Technology, Kanpur
Title of Thesis: *Hydrogen bond properties and dynamics of molecular solutions at ambient and non- ambient conditions: A computational study.*

2004-2006 Post doctoral research fellow, Georgetown University, Washington, DC

2006-2007 Post doctoral research fellow, University of Missouri St. Louis, Missouri, USA

Teaching Experience:

2007-2009 Lecturer, School of Chemistry and Biochemistry, Thapar University, Patiala, Punjab.

2009-Present Faculty, School of Basic Sciences, IIT Bhubaneswar, Odisha, India.

List of Publications:

34. R. Ghosh, A. Chakraborty, A. Biswas, S. Chowdhuri "Evaluation of Green Tea Polyphenols as Novel Corona Virus (SARS CoV-2) Main Protease (Mpro) Inhibitors – An In Silico/ Docking and Molecular Dynamics Simulation Study", *Journal of Biomolecular Structure & Dynamics*, 2020 (*in press*, DOI: 10.1080/07391102.2020.1779818)

33. P. Chettiyankandy, R. Ghosh, S. Chowdhuri, "Effects of concentration and pressure on the aqueous solvation structure of ammonia and composition dependent ion solvation scenario in water-ammonia mixtures," *Fluid Phase Equilibria*, 511, 112507 (2020).

32. P. Chettiyankandy, A. Chand, R. Ghosh, S.K. Sarkar, P. Das, S. Chowdhuri, "Effects of hexamethylenetetramine (HMTA) on the aqueous solution structure, dynamics and ion solvation scenario: A concentration and temperature dependent study with potential HMTA models", *J. Mol, Liq*., 296,111820 (2019).

31. P. Chettiyankandy,S. Chowdhuri, "Ion solvation scenario in an aqueous solution mixture of counteracting osmolytes: Urea and trimethylamine-N-oxide (TMAO). *J. Mol, Liq*., 293,111467 (2019).

30. A. Chand and S. Chowdhuri, "Pressure effects on solvation structure and dynamics in mixture of cis and trans- N-methylformamide in a protic and aprotic polar solvent", *J. Indian. Chem. Soc.* 96, 895 (2019).

29. A Chand, P Chettiyankandy and S Chowdhuri, "Behaviour of cis- and trans- N-methyl formamide in liquid mixture: Dynamical properties at varying pressure and temperature, and ion solvation scenario", *J. Mol. Liq*. 269, 241 (2018).

28. A. Chand and S. Chowdhuri, "A comparative study of hydrogen bonding structure and dynamics in aqueous urea solution of amides with varying hydrophobicity: Effect of addition of trimethylamine N-oxide (TMAO)", *J. Mol. Liq.*, 242, 70 (2017).

27. A. Chand, P. Chettiyankandy, S. K. Pattanayak and S. Chowdhuri, "Effects of trimethylamine-N-oxide (TMAO) on aqueous N-methylacetamide solution: A comparison of different force fields of TMAO", *J. Mol. Liq.*, 225, 926 (2017).

26. A. Chand and S. Chowdhuri, "Behaviour of aqueous N-methylacetamide solution in presence of ethanol and 2,2,2 tri-fluroethanol: Hydrogen bonding structure and dynamics", *J. Mol. Liq*., 224, 1370 (2016).

25. A. Chand and S. Chowdhuri, "Effects of dimethyl-sulfoxide on the hydrogen bonding structure and dynamics in aqueous N-methylacetamide solution: A Molecular dynamics simulations study", *J. Chem. Sci*., 128, 991 (2016).

24. P. Chettiyankandy and S. Chowdhuri, "Solvation structure and dynamics of ions in concentrated urea solution," *J. Mol. Liq*., 216, 788 (2016).

23. S. K. Pattanayak, P.Chettiyankandy and S. Chowdhuri, "Effects of co-solutes on the hydrogen bonding structure and dynamics in aqueous N-methylacetamide solution: A molecular dynamics study", *Mol. Phys*., 112, 2906 (2014).

22. S. K. Pattanayak and S. Chowdhuri, "Effects of methanol on the hydrogen bonding structure and dynamics in aqueous N-methylacetamide solution", *J. Mol. Liq*. 194, 141 (2014).

21. S. K. Pattanayak and S. Chowdhuri ," Dynamics of N-methylacetamide in water-ethanol mixtures of varying composition," *ISRAPS Bulletin* 25, 96 (2013).

20. S. K. Pattanayak and S. Chowdhuri, "Effects of concentrated NaCl and KCl solutions on the behaviour of aqueous peptide bond environment: single-particle dynamics and H-bond structural relaxation", *Mol. Phys*. 111, 3297 (2013).

19. S. K. Pattanayak and S. Chowdhuri, "Pressure and temperature dependence on the hydrogen bonding and dynamics of ammonium ion in liquid water: A molecular dynamics simulations study", *J. Mol. Liq*. 186, 98 (2013).

18. S. Chowdhuri and S. K. Pattanayak "Pressure effects on the dynamics of ions and solvent molecules in liquid methanol under ambient and cold conditions: Importance of solvent's H-bonding network", *J. Mol. Liq*. 180, 172 (2013).

17. S. Chowdhuri and S. K. Pattanayak "Pressure dependence on the single-particle dynamics and hydrogen bond structural relaxation of water-DMSO mixtures under ambient and cold conditions", *Mol. Phys.* 111, 135 (2013).

16. S. K. Pattanayak and S. Chowdhuri "A molecular dynamics simulations study on the behavior of liquid N-methylacetamide in presence of NaCl: Structure, dynamics and H-bond properties", *J. Mol. Liq*. 172, 102 (2012).

15. S. K. Pattanayak and S. Chowdhuri, "Size dependence of solvation structure and dynamics of ions in liquid N-methyl acetamide", *J. Theor. Comput. Chem*. 11(2), 361 (2012).

14. S. K. Pattanayak and S. Chowdhuri "Effect of water on solvation structure and dynamics of ions in peptide bond environment: Importance of hydrogen bonding and dynamics of the solvents", *J. Phys. Chem. B*, 115, 13241 (2011).

13. S. K. Pattanayak, N. Prashar and S. Chowdhuri, "Effect of temperature and pressure on the structure, dynamics and hydrogen bond properties of liquid N-methyl acetamide: A molecular dynamics study", *J. Chem. Phys*. 134, 154506 (2011).

12. S. Chowdhuri, D. Chakrobarty and A. Chandra, "Pressure effects on diffusion in liquid ammonia: A simulation study using a combination of isobaric-isothermal and micro-canonical molecular dynamics", *Indian J. Phys*. 83, 87 (2009).

11. S. Chowdhuri, M.-L. Tan, and T. Ichiye, "Dynamical properties of the SSDQO water model: A Molecular dynamics study", *J. Chem. Phys*. 125, 144513 (2006).

10. S. Chowdhuri and A. Chandra,"Dynamics of halide ion-water hydrogen bonds in aqueous solutions: Dependence on ion size and temperature", *J. Phys. Chem. B*, 110, 9674 (2006).

9. S. Chowdhuri and A. Chandra,"Solute size effects on the solvation structure and diffusion of ions in liquid methanol under normal and cold conditions", *J. Chem. Phys*., 124, 084507 (2006).

8. S. Chowdhuri and A. Chandra, "Dynamics of ionic and hydrophobic solutes in water-methanol mixtures of varying composition", *J. Chem. Phys.* 123, 234501 (2005).

7. S. Chowdhuri and A. Chandra, “Tracer diffusion of ionic and hydrophobic solutes in water-dimethyl sulfoxide mixtures: Effects of varying composition", *J. Chem. Phys*. 119, 4360 (2003).

6. S. Chowdhuri and A. Chandra, “Hydration structure and diffusion of ions in supercooled water: Ion size effects", *J. Chem. Phys.* 118, 9719 (2003).

5. S. Chowdhuri and A. Chandra, “Pressure effects on the tracer diffusion and orientational relaxation of hydrogen bonding solutes in ambient and supercooled water", *Chem. Phys. Lett*. 373, 79 (2003).

4. S. Chowdhuri and A. Chandra, “Hydrogen bonds in aqueous electrolyte solutions: Statistics and dynamics based on both geometric and energetic criteria", *Phys. Rev. E* 66, 041203 (2002).

3. A. Chandra and S. Chowdhuri, “Pressure effects on the dynamics and hydrogen bond properties of aqueous electrolyte solutions: The role of ion screening", *J. Phys. Chem. B*, 106, 6779 (2002).

2. A. Chandra and S. Chowdhuri, “Effects of hydrogen-bond environment on single particle and pair dynamics in liquid water", *Proc. Indian Acad. Sci. (Chem.Sci.)* 113, 591 (2001).

1. S. Chowdhuri and A. Chandra, “Moleculer dynamics simulations of aqueous NaCl and KCl solutions: Effects of ion concentration on the single-particle, pair and collective dynamical properties of ions and water molecules", *J. Chem. Phys*. 115, 3732 (2001).

Paper published in Conference:

1. P.Chettiyankany, A. Chand and S. Chowdhuri, “Effects of concentration and temperature on the solvation structure and dynamics of ions in aqueous Hexamethylenetetramine solution”, Souvenir : Seventh DAE-BRNS Symposium on Emerging Trends in Separation Science and Technology, pp.30-38, IIT Guwahati, 2016.

2. A. Chand, P. Chettiyankandy and S. Chowdhuri, Application of Computer Simulation in Exploring Influence of Alcohol on Aqueous Milieu of a Gut-Brain Octapeptide, Cholecystokinin-8. Soft Computing for Problem Solving. Advances in Intelligent Systems and Computing, pp. 25-40, vol. 817, 2019, Springer, Singapore (https://doi.org /10.1007/978-981-13-1595-4_3).

Book Chapter:

Molecular Basis and Emerging Strategies for Anti-aging Interventions Chapter 12: Computational Methods for developing Novel Anti-Aging Interventions, A. Chand, P. Chatteiyankandy, M. Moharana, S. N. Sahu, S. K. Pradhan, S. K Pattanayak, S. P. Mahapatra, A. Bissoyi, A. K. Singh and S. Chowdhuri, Springer, Singapore, Edition number 1, 2018 (DOI: 10.1007/978-981-13-1699-9).

Details of Projects (ongoing/completed):

1. Evaluation of natural polyphenols and nucleoside analogues compounds as novel corona virus (SARS CoV-2) main protease (Mpro/ 3CLpro) inhibitors – An in silico docking and molecular dynamics simulation study. IIT Delhi, 2020 (Co-PI: Dr. A. Biswas).
   (*Special call on high performance computation support by IIT Delhi for COVID-19 research*)
2. Influence of osmolytes on the structure, dynamics and hydrogen bond properties of water in aqueous solution and other aqueous binary mixtures at different thermo- dynamic conditions. DST-SERB, 2013-2016.
3. Structure and dynamics of ionic and molecular solutes in aqueous and non-aqueous solvents and in their binary mixture at different thermo- dynamic conditions: A molecular dynamics simulations study. CSIR, 2010-2013.