List of Publications of Dr. Sanjoy Bandyopadhyay

1) *Understanding the microscopic origin behind heterogeneous properties of water confined in and around $A\beta_{17-42}$ protofilaments.* P. Khatua and **S. Bandyopadhyay** *J. Chem. Phys.* (2018; in press).

2) *Dynamical crossover of water confined within the amphiphilic nanocores of aggregated amyloid β peptides.* P. Khatua and **S. Bandyopadhyay** *Phys. Chem. Chem. Phys. B* (2018; in press).

3) *Operation of Kelvin effect in the activities of an antifreeze protein: A molecular dynamics simulation study*. U. S. Midya and **S. Bandyopadhyay** *J. Phys. Chem. B* **122**, 3079-3087 (2018).

4) *Hydration behavior along the folding pathways of Trpzip4, Trpzip5 and Trpzip6*. M. Gupta, P. Khatua, C. Chakravarty and **S. Bandyopadhyay** *J. Phys. Chem. B* **122**, 1560-1572 (2018).

5) *Microscopic understanding of the conformational features of a protein-DNA complex*. S. Mondal, K. Chakraborty and **S. Bandyopadhyay** *Phys. Chem. Chem. Phys.* **19**, 32459-32472 (2017).

6) *Size-dependent conformational features of Abeta(17-42) protofilaments from molecular simulation studies*. P. Khatua, S. K. Sinha and **S. Bandyopadhyay** *J. Chem. Inf. Model.* **57**, 2378-2392 (2017).

7) *Sensitivity of folding free energy landscapes of trpzips to mutations in the hydrophobic core*. M. Gupta, P. Khatua, C. Chakravarty and **S. Bandyopadhyay** *Phys. Chem. Chem. Phys.* **19**, 22813-22825 (2017).

8) *Interfacial water arrangement in the ice-bound state of an antifreeze protein: A molecular dynamics simulation study.* U. S. Midya and **S. Bandyopadhyay** *Langmuir* **33**, 5499-5510 (2017).

9) *Water structure around hydrophobic amino acid side chain analogs using different water models.* T. Hajari and S. Bandyopadhyay *J. Chem. Phys.* **146**, 225104 (2017).

10) *In-silico studies of the early stages of aggregation of $A\beta_{42}$ peptides.* P. Khatua and **S. Bandyopadhyay** *J. Chem. Sci.* **129**, 899-909 (2017).

11) *Comparison of hydration behaviour and conformational preferences of Trp-cage mini-protein in different rigid-body water models.* M. Gupta, D. Nayar, C. Chakravarty and **S. Bandyopadhyay** *Phys. Chem. Chem. Phys.* **18**, 32796-32813 (2016).

12) *Conformational features of $A\beta_{42}$ peptide monomer and its interaction with surrounding solvent.* P. Khatua, J. C. Jose, N. Sengupta and *S. Bandyopadhyay Phys. Chem. Chem. Phys.* **18,** 30144-30159 (2016).

13) *Sensitivity of protein glass transition to choice of water model for Trp-cage mini-protein.* M. Gupta, C. Chakravarty and **S. Bandyopadhyay** *J. Chem. Theory and Comput.* **12,** 5643-5655 (2016).

14) *Exploring ion induced folding of a single-stranded DNA oligomer from molecular dynamics studies.* K. Chakraborty, P. Khatua and **S. Bandyopadhyay**, *Phys. Chem. Chem. Phys.* **18**, 15899-15910 (2016).

15) *Thermodynamics of complex structures formed between single-stranded DNA oligomers and the KH domains of the far upstream element binding protein*. K. Chakraborty, S. K. Sinha and **S. Bandyopadhyay**, *J. Chem. Phys.* **144**, 205105 (2016).

16) *Effect of protein-DNA complex formation on the intermolecular vibrational density of states of interfacial water*. K. Chakraborty and **S. Bandyopadhyay**, *Phys. Chem. Chem. Phys.* **18**, 7780-7788 (2016).

17) *Excess entropy and crystallization in Stillinger-Weber and Lennard-Jones fluids.* D. Dhabal, A. H. Nguyen, M. Singh, P. Khatua V. Molinero, **S. Bandyopadhyay** and C. Chakravarty, *J. Chem. Phys.* **143**, 164512 (2015).

18) *Dynamics of water around the complex structures formed between the KH domains of Far Upstream Element binding protein and single-stranded DNA molecules.* K. Chakraborty and **S. Bandyopadhyay**, *J. Chem. Phys.* **143**, 045106 (2015).

19) *Correlated conformational motions of the KH domains of far upstream element binding protein complexed with single-stranded DNA oligomers.* K. Chakraborty and **S. Bandyopadhyay**, *J. Phys. Chem. B* **119**, 10998-11009 (2015).

20) *Microscopic dynamics of water around unfolded structures of barstar at room temperature.* S. Pal, K. Chakraborty, P. Khatua and **S. Bandyopadhyay**, *J. Chem. Phys.* **142**, 055102 (2015). **(Most Read article published in 2015 in *The J. Chem. Phys.*)**

21) *Effect of temperature on the low-frequency vibrational spectrum and relative structuring of hydration water around a single-stranded DNA.* K. Chakraborty and **S. Bandyopadhyay**, *J. Chem. Phys.* **142**, 015101 (2015). **(Most Read article published in 2015 in *The J. Chem. Phys.*)**

22) *Microscopic hydration properties of the ABeta(1-42) peptide monomer and the globular protein ubiquitin: A comparative molecular dynamics study*. J. C. Jose, P. Khatua, N. Bansal, N. Sengupta and **S. Bandyopadhyay**, *J. Phys. Chem. B* **118**, 11591-11604 (2014).

23) *In-silico studies of the properties of water hydrating a small protein*. S. K. Sinha, M. Jana, K. Chakraborty and **S. Bandyopadhyay**, *J. Chem. Phys.* **141**, 22D502 (2014).

24) *Hydration behavior at the ice-binding surface of the antifreeze protein TmAFP*. U. S. Midya and **S. Bandyopadhyay**, *J. Phys. Chem. B* **118**, 4743-4752 (2014).

25) *Correlated dynamical crossovers of the hydration layer of a single-stranded DNA oligomer.* K. Chakraborty and **S. Bandyopadhyay**, *J. Phys. Chem. B* **118**, 413-422 (2014).

26) *Thermal unfolding of barstar and the properties of interfacial water around the unfolded forms.* S. Pal and **S. Bandyopadhyay**, *J. Chem. Phys.* **139**, 235101 (2013).

27) *Molecular dynamics simulation of a single-stranded DNA with heterogeneous distribution of nucleobases in aqueous medium.* K. Chakraborty, S. Mantha and **S. Bandyopadhyay**, *J. Chem. Phys.* **139**, 075103 (2013).

28) *Molecular dynamics study of beta-cyclodextrin-phenylalanine (1:1) inclusion complex in aqueous medium*. M. Jana and **S. Bandyopadhyay**, *J. Phys. Chem. B* **117**, 9280-9287 (2013).

29) *Computer simulation studies of biomolecular hydration.* S. Pal, K. Chakraborty, U. S. Midya, P. Khatua and **S. Bandyopadhyay**, *ISRAPS Bull.* **25**, 77-83 (2013).

30) *Effects of protein conformational motions in the native form and non-uniform distribution of electrostatic interaction sites on interfacial water*. S. Pal and **S. Bandyopadhyay**, *Chem. Phys.* **420**, 35-43 (2013).

31) *Effects of protein conformational flexibilities and electrostatic interactions on the low-frequency vibrational spectrum of hydration water*. S. Pal and **S. Bandyopadhyay**, *J. Phys. Chem. B* **117**, 5848-5856 (2013).

32) *Importance of protein conformational motions and electrostatic anchoring sites on the dynamics and hydrogen bond properties of hydration water*. S. Pal and **S. Bandyopadhyay**, *Langmuir* **29**, 1162-1173 (2013).

33) *Restricted dynamics of water around a protein-carbohydrate complex: Computer simulation studies*. M. Jana and **S. Bandyopadhyay**, *J. Chem. Phys.* **137**, 055102 (2012).

34) *Polar solvation dynamics of lysozyme from molecular dynamics studies*. S. K. Sinha and **S. Bandyopadhyay**, *J. Chem. Phys.* **136**, 185102 (2012).

    This article has been selected for publication in *Virtual Journal of Biological Physics Research* **23** (January 1, 2012).

35) *Conformational flexibility of a protein-carbohydrate complex and the structure and ordering of surrounding water*. M. Jana and S. Bandyopadhyay, *Phys. Chem. Chem. Phys.* **14**, 6628-6638 (2012).

36) *Local heterogeneous dynamics of water around lysozyme: A computer simulation study*. S. K. Sinha and **S. Bandyopadhyay**, *Phys. Chem. Chem. Phys.* **14**, 899-913 (2012).

37) *Conformational fluctuations of a protein-DNA complex and the structure and ordering of water around it.* S. K. Sinha and **S. Bandyopadhyay**, *J. Chem. Phys.* **135**, 245104 (2011).

This article has been selected for publication in *JCP: BioChemical Physics* **5** (December, 2011), and in *Virtual Journal of Biological Physics Research* **23** (January 1, 2012).

38) *Dynamical properties of water around a protein-DNA complex form molecular dynamics simulations.* S. K. Sinha and **S. Bandyopadhyay** *J. Chem. Phys.* **(cover page) 135**, 135101 (2011).

One of the **Top 20** Most Downloaded Articles in October 2011.
This article has been selected for publication in *JCP: BioChemical Physics* **5** (October, 2011), and in *Virtual Journal of Biological Physics Research* **21** (October 15, 2011).

39) *Vibrational spectrum of water confined in and around cyclodextrins.* M. Jana and **S. Bandyopadhyay** *Chem. Phys. Lett.* **509**, 181-185 (2011).

40) *Hydration Properties of α-, β-, and γ-cyclodextrins from molecular dynamics simulations.* M. Jana and **S. Bandyopadhyay** *J. Phys. Chem. B* **115,** 6347-6357 (2011).

41) *Differential flexibility of the secondary structures of lysozyme and the structure and ordering of surrounding water molecules*. S. K. Sinha and **S. Bandyopadhyay** *J. Chem. Phys.* **134**, 115101 (2011).

This article has been selected for publication in *JCP: BioChemical Physics* **5** (March, 2011), and in *Virtual Journal of Biological Physics Research* **21** (March 15, 2011).

42) *Kinetics of hydrogen bonds in aqueous solutions of cyclodextrin and its methyl-substituted forms*. M. Jana and **S. Bandyopadhyay** *J. Chem. Phys.* **134,** 025103 (2011).

This article has been selected for publication in *JCP: BioChemical Physics* **5** (January, 2011), and in *Virtual Journal of Biological Physics Research* **21** (January 15, 2011).

43) *Low-frequency vibrational spectrum of water around cyclodextrin and its methyl-substituted derivatives*. M. Jana and **S. Bandyopadhyay** *Langmuir* **26,** 14097-14102 (2010).

44) *Secondary structure specific entropy change of a partially unfolded protein molecule*. S. K. Sinha, S. Chakraborty and **S. Bandyopadhyay** *Langmuir* **26,** 9911-9916 (2010).

45) *Microscopic investigation of the hydration properties of cyclodextrin and its substituted forms*. M. Jana and **S. Bandyopadhyay** *Langmuir* **25,** 13084-13091 (2009).

46) *Effect of unfolding on the thickness of the hydration layer of a protein*. S. K. Sinha, S. Chakraborty and **S. Bandyopadhyay** *Ind. J. Phys.* **83**, 49-64 (2009).

47) *Thickness of the hydration layer of a protein from molecular dynamics simulation*. S. K. Sinha, S. Chakraborty and **S. Bandyopadhyay** *J. Phys. Chem. B* **112**, 8203-8209 (2008).

48) *Dynamics of water in the hydration layer of a partially unfolded structure of the protein HP-36*. S. Chakraborty and **S. Bandyopadhyay** *J. Phys. Chem. B* **112**, 6500-6507 (2008).

49) *Low-frequency vibrational spectrum of water in the hydration layer of a protein: A molecular dynamics simulation study*. S. Chakraborty, S. K. Sinha and **S. Bandyopadhyay** *J. Phys. Chem. B* **111**, 13626-13631 (2007).

50) *Correlation between the dynamics of hydrogen bonds and the local density reorganization in the protein hydration layer*. S. Chakraborty and **S. Bandyopadhyay**, *J. Phys. Chem. B* **111**, 7626-7630 (2007).

51) *Molecular dynamics study of surfactant monolayers adsorbed at the oil/water and air/water interfaces*. J. Chanda and **S. Bandyopadhyay**, *J. Phys. Chem. B* **110**, 23482-23488 (2006).

52) *Hydrogen bond lifetime dynamics at the interface of a surfactant monolayer*. J. Chanda and **S. Bandyopadhyay**, *J. Phys. Chem. B* **110**, 23443-23449 (2006).

53) *Exploration of the secondary structure specific differential solvation dynamics between the native and molten globule states of the protein HP-36*. **S. Bandyopadhyay**, S. Chakraborty and B. Bagchi, *J. Phys. Chem. B* **110**, 20629-20634 (2006).

54) *Water dynamics at the surface of proteins and micelles: Understanding the fast and the slow components*. S. Pal, S. Chakraborty, S. M. Bhattacharyya, **S. Bandyopadhyay**, S. Balasubramanian and B. Bagchi, in *Water Properties of Food, Pharmaceutical, and Biological Materials*, Eds. M. D. P. Buera, J. Welti-Chanes, P. J. Lillford and H. R. Corti, Taylor and Francis Publisher, p.11-37 (2006).

55) *Coupling between hydration layer dynamics and unfolding kinetics of HP-36*. **S. Bandyopadhyay**, S. Chakraborty and B. Bagchi, *J. Chem. Phys.* **125**, 084912 (2006).

This article has been selected for publication in *Virtual Journal of Biological Physics Research* **12** (September 1, 2006).

56) *Perturbation of phospholipid bilayer properties by ethanol at a high concentration*. J. Chanda and **S. Bandyopadhyay**, *Langmuir* **22**, 3775-3781 (2006).

57) *Sensitivity of hydrogen bond lifetime dynamics to the presence of ethanol at the interface of a phospholipid bilayer*. J. Chanda, S. Chakraborty and **S. Bandyopadhyay**, *J. Phys. Chem. B* **110**, 3791-3797 (2006).

58) *Secondary structure sensitivity of hydrogen bond lifetime dynamics in the protein hydration layer*. **S. Bandyopadhyay**, S. Chakraborty and B. Bagchi, *J. Am. Chem. Soc.* **127**, 16660-16667 (2005).

59) *Correlation between the dynamics of amino acid residues and water molecules in aqueous protein solutions*. **S. Bandyopadhyay**, *Abstr. Pap. Am. Chem. Soc*. **229**, 335-COMP Part 1 (March, 2005).

60) *Molecular dynamics study of a surfactant monolayer adsorbed at air/water interface*. J. Chanda and **S. Bandyopadhyay**, *J. Chem. Theory and Comput.* **1**, 963-971 (2005).

61) *Bimodal water dynamics at the surface of micelles and proteins*. S. Balasubramanian, S. Chakraborty, **S. Bandyopadhyay**, S. Pal and B. Bagchi, *Ultrafast Phenomena XIV* (Proceedings of the 14th International Conference) Eds. T. Kobayashi, T. Okada, T. Kobayashi, K. A. Nelson and S. De Silvestri, Springer Series in Chemical Physics, v.79 (2005).

62) *Sensitivity of polar solvation dynamics to the secondary structures of aqueous proteins and the role of surface exposure of the probe*. **S. Bandyopadhyay**, S. Chakraborty, S. Balasubramanian and B. Bagchi, *J. Am. Chem. Soc.* **127**, 4071-4075 (2005).

63) *Monolayer of Aerosol-OT surfactants adsorbed at the air/water interface: An atomistic computer simulation study*. J. Chanda, S. Chakraborty and **S. Bandyopadhyay**, *J. Phys. Chem. B* **109**, 471-479 (2005).

64) *Molecular modeling and simulations of AOT-water reverse micelles in iso-octane: Structural and dynamical properties*. S. Abel, F. Sterpone, **S. Bandyopadhyay** and M. Marchi, *J. Phys. Chem. B* **108**, 19458-19466 (2004).

65) *Atomistic simulation study of the coupled motion of amino acid residues and water molecules around protein HP-36 : Fluctuations at and around the active sites*. **S. Bandyopadhyay**, S. Chakraborty, S. Balasubramanian, S. Pal and B. Bagchi, *J. Phys. Chem. B* **108** 12608-12616 (2004).

66) *Distribution of ethanol in a model membrane: A computer simulation study*. J. Chanda and **S. Bandyopadhyay**, *Chem. Phys. Lett.* **392**, 249-254 (2004).

67) *Dynamics of water at surface of complex systems: Study of aqueous micelles and proteins*. S. Pal, **S. Bandyopadhyay**, S. Balasubramanian and B. Bagchi, in

Femtochemistry and Femtobiology: *Ultrafast Events in Molecular Science*, Ed. M. M. Martin and J. T. Hynes, Elsevier Publisher (ISBN: 0444516565), p.213-220 (2004).

68) *Effect of the pore region of a transmembrane ion-channel on the physical properties of a simple membrane*. L. Saiz, **S. Bandyopadhyay** and M. L. Klein, *J. Phys. Chem. B* **108**, 2608-2613 (2004).

69) *Dynamics of water at the interface of a small protein, enterotoxin*. S. Balasubramanian, **S. Bandyopadhyay**, S. Pal and B. Bagchi, *Curr. Sci.* **85**, 101-108 (2003).

70) *Effect of the pore region of a transmembrane ion-channel on the physical properties of a simple membrane*. L. Saiz, **S. Bandyopadhyay** and M. L. Klein, *Biophys J.* **84** (2), 382A-382A Part 2 Suppl. S (February, 2003).

71) *Monolayer of monododecyl diethylene glycol surfactants adsorbed at the air/water interface* : *A molecular dynamics study*. **S. Bandyopadhyay** and J. Chanda, *Langmuir* **19**, 10443-10448 (2003).

72) *Computer simulation studies of surfactant assemblies and complex biological systems*. **S. Bandyopadhyay**, *Res. and Innovation* **11**, 21-25 (2003).

73) *Effects of the nonimmobilizer hexafluoroethane on the model membrane dimyristoylphosphatidylcholine*. L. Koubi, M. Tarek, **S. Bandyopadhyay**, M. L. Klein and D Scharf, *Anesthesiology* **97**, 848-855 (2002).

74) *Towards an understanding of complex biological membranes from atomistic molecular dynamics simulations*. L. Saiz, **S. Bandyopadhyay** and M. L. Klein, *Bioscience Reports* **22**, 151-173 (2002).

75) *Membrane structural perturbations caused by anesthetics and non-immobilizers* : *A molecular dynamics investigation*. L. Koubi, M. Tarek, **S. Bandyopadhyay**, M. L. Klein and D Scharf, *Biophys. J.* **81**, 3339-3345 (2001).

76) *Simulations of phospholipids using a coarse grain model*. J. C. Shelley, M. Y. Shelley, R. C. Reeder, **S. Bandyopadhyay**, P. B. Moore and M. L. Klein, *J. Phys. Chem. B* **105**, 9785-9792 (2001).

77) *Comparing non-immobilizer to anesthetic distribution in a model membrane*. D. Scharf, L. Koubi, M. Tarek, **S. Bandyopadhyay** and M. L. Klein, *Biophys J.* **80 (1)**, 2154 Part 2, (January, 2001).

78) *Molecular dynamics study of the effect of surfactant on a biomembrane*. **S. Bandyopadhyay**, J. C. Shelley and M. L. Klein, *J. Phys. Chem. B* **105**, 5979-5986 (2001).

79) *Molecular dynamics simulation studies of surfactant systems*. R. Allen, **S. Bandyopadhyay**, J. C. Shelley, M. Y. Shelley and M. L. Klein, *Abstr. Pap. Am. Chem. Soc.* **221**, 15-Coll Part 1 (April, 2001).

80) *A coarse grain model for phospholipid simulations*. J. C. Shelley, M. Y. Shelley, R. C. Reeder, **S. Bandyopadhyay** and M. L. Klein, *J. Phys. Chem. B* **105**, 4464-4470 (2001).

81) *$C_{12}E_2$ reverse micelle*: *A molecular dynamics study*. R. Allen, **S. Bandyopadhyay** and M. L. Klein, *Langmuir* **16**, 10547-10552 (2000).

82) *Molecular dynamics study of the poly(oxyethylene) surfactant $C_{12}E_2$ and water*. **S. Bandyopadhyay**, M. Tarek, M. Lynch and M. L. Klein, *Langmuir* **16**, 942-946 (2000).

83) *Computer simulation studies of surfactant systems*. **S. Bandyopadhyay**, M. Tarek and M. L. Klein, in *New Approaches to Problems in Liquid State Theory*, Ed. C. Caccamo, J.-P. Hansen and G. Stell, Kluwer Academic Publishers, Netherlands, v. 529, 347-354 (1999).

84) *Molecular dynamics study of a lipid-DNA complex*. **S. Bandyopadhyay**, M. Tarek and M. L. Klein, *J. Phys. Chem. B* **103**, 10075-10080 (1999).

85) *Molecular dynamics studies of the hexagonal mesophase of sodium dodecylsulphate in aqueous solution*. **S. Bandyopadhyay**, M. L. Klein, G. J. Martyna, and M. Tarek, *Mol. Phys.* **95**, 377-384 (1998).

86) *Molecular dynamics studies of aqueous surfactants systems*. M. Tarek, **S. Bandyopadhyay**, and M. L. Klein, *J. Mol. Liqs.* **78**, 1-6 (1998).

87) *Surfactant aggregation at a hydrophobic surface*. **S. Bandyopadhyay**, J. C. Shelley, M. Tarek, P. B. Moore, and M. L. Klein, *J. Phys. Chem. B* **102**, 6318-6322 (1998).

88) *Computer simulation studies of amphiphilic interfaces*. **S. Bandyopadhyay**, M. Tarek, and M. L. Klein, *Curr. Opin. Colloid & Interface Sci.* **3**, 242-246 (1998).

89) *Effect of variation of the size of CH_3 and CH_2 groups on cage-to-cage migration of n-butane in zeolite NaCaA*. **S. Bandyopadhyay**, *Chem. Phys. Lett.* **293**, 378-382 (1998).

90) *Conformational analysis of n-butane in zeolite NaCaA: Temperature and concentration dependence*. **S. Bandyopadhyay** and S. Yashonath, *J. Phys. Chem. B* **101**, 5675-5683 (1997).

91) *A Monte Carlo method for estimation of pore volumes of zeolites*. **S. Bandyopadhyay** and S. Yashonath, *Zeolites* **19**, 51-56 (1997).

92) *Monte Carlo and molecular dynamics simulation of argon clusters and n-alkanes in the confined regions of zeolites*. R. Chitra, **S. Bandyopadhyay** and S. Yashonath, *Bull. Mater. Sci.* **20**, 845-878 (1997).

93) *Conformation of confined alkanes: n-butane in zeolite Y*. **S. Bandyopadhyay** and S. Yashonath, *J. Chem. Phys.* **105**, 7223-7226 (1996).

94) *Diffusion anomaly in silicalite and VPI-5 from molecular dynamics simulations*. **S. Bandyopadhyay** and S. Yashonath, *J. Phys. Chem.* **99**, 4286-4292 (1995).

95) *Surprising diffusion behaviour in the restricted regions of Silicalite*. S. Yashonath and **S. Bandyopadhyay**, *Chem. Phys. Lett.* **228**, 284-288 (1994).

96) *Sorbate properties of xenon in Cloverite: A molecular dynamics study*. **S. Bandyopadhyay** and S. Yashonath, *J. Solid State Chem.* **111**, 151-156 (1994).

97) *CHIPPS: A data parallel computer for analysis of molecular dynamics trajectories*. **S. Bandyopadhyay**, S. Yashonath, T. C. Subramanian and M. Periasamy, *Trans. Mat. Res. Soc. Jpn.* **16A**, 157, (1994).

98) *Anomalous behaviour of cage-to-cage diffusion of methane in zeolites A and Y*. **S. Bandyopadhyay** and S. Yashonath, *Chem. Phys. Lett.* **223**, 363-368 (1994).