

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 β 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).
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