Sanjoy Bandyopadhyay

List of Publications by Year
in descending order

68	1,587	279798 23	330143 37
papers	citations	h-index	g-index

68	68	68	1480
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dynamic Heterogeneity at the Interface of an Intrinsically Disordered Peptide. Journal of Chemical Information and Modeling, 2022, 62, 1942-1955.	5.4	6
2	Exploring Heterogeneous Dynamical Environment around an Ensemble of AÎ²₄₂ Peptide Monomer Conformations. Journal of Chemical Information and Modeling, 2022, 62, 3453-3462.	5.4	4
3	Contrasting Effects of Ionic Liquids of Varying Degree of Hydrophilicity on the Conformational and Interfacial Properties of a Globular Protein. Journal of Physical Chemistry B, 2021, 125, 9441-9453.	2.6	6
4	Importance of Solvent in Guiding the Conformational Properties of an Intrinsically Disordered Peptide. Langmuir, 2021, 37, 14429-14442.	3.5	5
5	Effect of aggregated AÎ²Âprotofilaments on intermolecular vibrational spectrum of confined water. Journal of Chemical Sciences, 2020, 132, 1.	1.5	2
6	Microscopic Understanding of the Effect of Ionic Liquid on Protein from Molecular Simulation Studies. Journal of Physical Chemistry B, 2020, 124, 3909-3921.	2.6	20
7	Heterogeneous Dynamical Environment at the Interface of a Proteinâ€“DNA Complex. Langmuir, 2020, 36, 4567-4581.	3.5	3
8	Intermolecular Dynamics of Water: Suitability of Reactive Interatomic Potential. Journal of Physical Chemistry B, 2019, 123, 6529-6535.	2.6	9
9	Flexibility of the Binding Regions of a Proteinâ€“DNA Complex and the Structure and Ordering of Interfacial Water. Journal of Chemical Information and Modeling, 2019, 59, 4427-4437.	5.4	4
10	Effects of Metal Ions on AÎ²₄₂ Peptide Conformations from Molecular Simulation Studies. Journal of Chemical Information and Modeling, 2019, 59, 2879-2893.	5.4	15
11	Operation of Kelvin Effect in the Activities of an Antifreeze Protein: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2018, 122, 3079-3087.	2.6	16
12	Hydration Behavior along the Folding Pathways of Trpzip4, Trpzip5 and Trpzip6. Journal of Physical Chemistry B, 2018, 122, 1560-1572.	2.6	6
13	Role of Polar and Nonpolar Groups in the Activity of Antifreeze Proteins: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2018, 122, 9389-9398.	2.6	11
14	Dynamical crossover of water confined within the amphiphilic nanocores of aggregated amyloid Î² peptides. Physical Chemistry Chemical Physics, 2018, 20, 14835-14845.	2.8	13
15	Understanding the microscopic origin behind heterogeneous properties of water confined in and around AÎ²17â€“42 protofilaments. Journal of Chemical Physics, 2018, 149, 065101.	3.0	7
16	In silico studies of the early stages of aggregation of A $$eta _{42}$$ Î² 42 Âpeptides. Journal of Chemical Sciences, 2017, 129, 899-909.	1.5	5
17	Water structure around hydrophobic amino acid side chain analogs using different water models. Journal of Chemical Physics, 2017, 146, 225104.	3.0	18
18	Interfacial Water Arrangement in the Ice-Bound State of an Antifreeze Protein: A Molecular Dynamics Simulation Study. Langmuir, 2017, 33, 5499-5510.	3.5	23

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19	Size-Dependent Conformational Features of AÎ²_{17â€“42} Protofilaments from Molecular Simulation Studies. Journal of Chemical Information and Modeling, 2017, 57, 2378-2392.	5.4	12
20	The sensitivity of folding free energy landscapes of trpzips to mutations in the hydrophobic core. Physical Chemistry Chemical Physics, 2017, 19, 22813-22825.	2.8	5
21	Microscopic understanding of the conformational features of a proteinâ€“DNA complex. Physical Chemistry Chemical Physics, 2017, 19, 32459-32472.	2.8	3
22	Thermodynamics of complex structures formed between single-stranded DNA oligomers and the KH domains of the far upstream element binding protein. Journal of Chemical Physics, 2016, 144, 205105.	3.0	4
23	Comparison of hydration behavior and conformational preferences of the Trp-cage mini-protein in different rigid-body water models. Physical Chemistry Chemical Physics, 2016, 18, 32796-32813.	2.8	16
24	Conformational features of the AÎ²₄₂ peptide monomer and its interaction with the surrounding solvent. Physical Chemistry Chemical Physics, 2016, 18, 30144-30159.	2.8	25
25	Sensitivity of Protein Glass Transition to the Choice of Water Model. Journal of Chemical Theory and Computation, 2016, 12, 5643-5655.	5.3	16
26	Exploring ion induced folding of a single-stranded DNA oligomer from molecular simulation studies. Physical Chemistry Chemical Physics, 2016, 18, 15899-15910.	2.8	18
27	Effects of proteinâ€“DNA complex formation on the intermolecular vibrational density of states of interfacial water. Physical Chemistry Chemical Physics, 2016, 18, 7780-7788.	2.8	4
28	Excess entropy and crystallization in Stillinger-Weber and Lennard-Jones fluids. Journal of Chemical Physics, 2015, 143, 164512.	3.0	34
29	Dynamics of water around the complex structures formed between the KH domains of far upstream element binding protein and single-stranded DNA molecules. Journal of Chemical Physics, 2015, 143, 045106.	3.0	11
30	Correlated Conformational Motions of the KH Domains of Far Upstream Element Binding Protein Complexed with Single-Stranded DNA Oligomers. Journal of Physical Chemistry B, 2015, 119, 10998-11009.	2.6	7
31	Effect of temperature on the low-frequency vibrational spectrum and relative structuring of hydration water around a single-stranded DNA. Journal of Chemical Physics, 2015, 142, 015101.	3.0	3
32	Microscopic dynamics of water around unfolded structures of barstar at room temperature. Journal of Chemical Physics, 2015, 142, 055102.	3.0	14
33	In silico studies of the properties of water hydrating a small protein. Journal of Chemical Physics, 2014, 141, 22D502.	3.0	20
34	Correlated Dynamical Crossovers of the Hydration Layer of a Single-Stranded DNA Oligomer. Journal of Physical Chemistry B, 2014, 118, 413-422.	2.6	12
35	Hydration Behavior at the Ice-Binding Surface of the Tenebrio molitor Antifreeze Protein. Journal of Physical Chemistry B, 2014, 118, 4743-4752.	2.6	39
36	Microscopic Hydration Properties of the AÎ²_{1â€“42} Peptide Monomer and the Globular Protein Ubiquitin: A Comparative Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 11591-11604.	2.6	15

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37	Molecular dynamics simulation of a single-stranded DNA with heterogeneous distribution of nucleobases in aqueous medium. Journal of Chemical Physics, 2013, 139, 075103.	3.0	28
38	Effects of protein conformational motions in the native form and non-uniform distribution of electrostatic interaction sites on interfacial water. Chemical Physics, 2013, 420, 35-43.	1.9	10
39	Thermal unfolding of barstar and the properties of interfacial water around the unfolded forms. Journal of Chemical Physics, 2013, 139, 235101.	3.0	6
40	Effects of Protein Conformational Flexibilities and Electrostatic Interactions on the Low-Frequency Vibrational Spectrum of Hydration Water. Journal of Physical Chemistry B, 2013, 117, 5848-5856.	2.6	22
41	Importance of Protein Conformational Motions and Electrostatic Anchoring Sites on the Dynamics and Hydrogen Bond Properties of Hydration Water. Langmuir, 2013, 29, 1162-1173.	3.5	44
42	Local heterogeneous dynamics of water around lysozyme: a computer simulation study. Physical Chemistry Chemical Physics, 2012, 14, 899-913.	2.8	35
43	Hydration Properties of Î±-, Î²-, and Î³-Cyclodextrins from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 6347-6357.	2.6	39
44	Conformational fluctuations of a proteinâ€“DNA complex and the structure and ordering of water around it. Journal of Chemical Physics, 2011, 135, 245104.	3.0	11
45	Dynamic properties of water around a proteinâ€“DNA complex from molecular dynamics simulations. Journal of Chemical Physics, 2011, 135, 135101.	3.0	37
46	Kinetics of hydrogen bonds in aqueous solutions of cyclodextrin and its methyl-substituted forms. Journal of Chemical Physics, 2011, 134, 025103.	3.0	19
47	Vibrational spectrum of water confined in and around cyclodextrins. Chemical Physics Letters, 2011, 509, 181-185.	2.6	9
48	Differential flexibility of the secondary structures of lysozyme and the structure and ordering of surrounding water molecules. Journal of Chemical Physics, 2011, 134, 115101.	3.0	28
49	Low-Frequency Vibrational Spectrum of Water around Cyclodextrin and Its Methyl-Substituted Derivatives. Langmuir, 2010, 26, 14097-14102.	3.5	13
50	Secondary Structure Specific Entropy Change of a Partially Unfolded Protein Molecule. Langmuir, 2010, 26, 9911-9916.	3.5	8
51	Effect of unfolding on the thickness of the hydration layer of a protein. Indian Journal of Physics, 2009, 83, 49-64.	1.8	1
52	Microscopic Investigation of the Hydration Properties of Cyclodextrin and Its Substituted Forms. Langmuir, 2009, 25, 13084-13091.	3.5	23
53	Thickness of the Hydration Layer of a Protein from Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 8203-8209.	2.6	55
54	Dynamics of Water in the Hydration Layer of a Partially Unfolded Structure of the Protein HP-36. Journal of Physical Chemistry B, 2008, 112, 6500-6507.	2.6	16

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55	Low-Frequency Vibrational Spectrum of Water in the Hydration Layer of a Protein:Â A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 13626-13631.	2.6	40
56	Correlation between the Dynamics of Hydrogen Bonds and the Local Density Reorganization in the Protein Hydration Layer. Journal of Physical Chemistry B, 2007, 111, 7626-7630.	2.6	24
57	Perturbation of Phospholipid Bilayer Properties by Ethanol at a High Concentration. Langmuir, 2006, 22, 3775-3781.	3.5	39
58	Molecular Dynamics Study of Surfactant Monolayers Adsorbed at the Oil/Water and Air/Water Interfaces. Journal of Physical Chemistry B, 2006, 110, 23482-23488.	2.6	86
59	Exploration of the Secondary Structure Specific Differential Solvation Dynamics between the Native and Molten Globule States of the Protein HP-36. Journal of Physical Chemistry B, 2006, 110, 20629-20634.	2.6	18
60	Sensitivity of Hydrogen Bond Lifetime Dynamics to the Presence of Ethanol at the Interface of a Phospholipid Bilayerâ€. Journal of Physical Chemistry B, 2006, 110, 3791-3797.	2.6	53
61	Coupling between hydration layer dynamics and unfolding kinetics of HP-36. Journal of Chemical Physics, 2006, 125, 084912.	3.0	25
62	Sensitivity of Polar Solvation Dynamics to the Secondary Structures of Aqueous Proteins and the Role of Surface Exposure of the Probe. Journal of the American Chemical Society, 2005, 127, 4071-4075.	13.7	92
63	Molecular Dynamics Study of a Surfactant Monolayer Adsorbed at the Air/Water Interface. Journal of Chemical Theory and Computation, 2005, 1, 963-971.	5.3	87
64	Secondary Structure Sensitivity of Hydrogen Bond Lifetime Dynamics in the Protein Hydration Layer. Journal of the American Chemical Society, 2005, 127, 16660-16667.	13.7	137
65	Distribution of ethanol in a model membrane: a computer simulation study. Chemical Physics Letters, 2004, 392, 249-254.	2.6	23
66	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. Journal of Physical Chemistry B, 2004, 108, 12608-12616.	2.6	60
67	Molecular Dynamics Study of the Effect of Surfactant on a Biomembrane. Journal of Physical Chemistry B, 2001, 105, 5979-5986.	2.6	58
68	Monte Carlo and molecular dynamics simulation of argon clusters andn-alkanes in the confined regions of zeolites. Bulletin of Materials Science, 1997, 20, 845-878.	1.7	10