

Sanjoy Bandyopadhyay

List of Publications by Year in descending order

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279798

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docs citations

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times ranked

1480
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
3	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
4	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
5	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
6	Molecular Dynamics Study of the Effect of Surfactant on a Biomembrane. Journal of Physical Chemistry B, 2001, 105, 5979-5986.	2.6	58
7	Thickness of the Hydration Layer of a Protein from Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 8203-8209.	2.6	55
8	Sensitivity of Hydrogen Bond Lifetime Dynamics to the Presence of Ethanol at the Interface of a Phospholipid Bilayer. Journal of Physical Chemistry B, 2006, 110, 3791-3797.	2.6	53
9	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
10	Low-Frequency Vibrational Spectrum of Water in the Hydration Layer of a Protein: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 13626-13631.	2.6	40
11	Perturbation of Phospholipid Bilayer Properties by Ethanol at a High Concentration. Langmuir, 2006, 22, 3775-3781.	3.5	39
12	Hydration Properties of $\hat{1}$ -, $\hat{2}$ -, and $\hat{3}$ -Cyclodextrins from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 6347-6357.	2.6	39
13	Hydration Behavior at the Ice-Binding Surface of the <i>Tenebrio molitor</i> Antifreeze Protein. Journal of Physical Chemistry B, 2014, 118, 4743-4752.	2.6	39
14	Dynamic properties of water around a protein-DNA complex from molecular dynamics simulations. Journal of Chemical Physics, 2011, 135, 135101.	3.0	37
15	Local heterogeneous dynamics of water around lysozyme: a computer simulation study. Physical Chemistry Chemical Physics, 2012, 14, 899-913.	2.8	35
16	Excess entropy and crystallization in Stillinger-Weber and Lennard-Jones fluids. Journal of Chemical Physics, 2015, 143, 164512.	3.0	34
17	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
18	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

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19	Coupling between hydration layer dynamics and unfolding kinetics of HP-36. <i>Journal of Chemical Physics</i> , 2006, 125, 084912.	3.0	25
20	Conformational features of the A β 42 peptide monomer and its interaction with the surrounding solvent. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30144-30159.	2.8	25
21	Correlation between the Dynamics of Hydrogen Bonds and the Local Density Reorganization in the Protein Hydration Layer. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7626-7630.	2.6	24
22	Distribution of ethanol in a model membrane: a computer simulation study. <i>Chemical Physics Letters</i> , 2004, 392, 249-254.	2.6	23
23	Microscopic Investigation of the Hydration Properties of Cyclodextrin and Its Substituted Forms. <i>Langmuir</i> , 2009, 25, 13084-13091.	3.5	23
24	Interfacial Water Arrangement in the Ice-Bound State of an Antifreeze Protein: A Molecular Dynamics Simulation Study. <i>Langmuir</i> , 2017, 33, 5499-5510.	3.5	23
25	Effects of Protein Conformational Flexibilities and Electrostatic Interactions on the Low-Frequency Vibrational Spectrum of Hydration Water. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5848-5856.	2.6	22
26	In silico studies of the properties of water hydrating a small protein. <i>Journal of Chemical Physics</i> , 2014, 141, 22D502.	3.0	20
27	Microscopic Understanding of the Effect of Ionic Liquid on Protein from Molecular Simulation Studies. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3909-3921.	2.6	20
28	Kinetics of hydrogen bonds in aqueous solutions of cyclodextrin and its methyl-substituted forms. <i>Journal of Chemical Physics</i> , 2011, 134, 025103.	3.0	19
29	Exploration of the Secondary Structure Specific Differential Solvation Dynamics between the Native and Molten Globule States of the Protein HP-36. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20629-20634.	2.6	18
30	Exploring ion induced folding of a single-stranded DNA oligomer from molecular simulation studies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15899-15910.	2.8	18
31	Water structure around hydrophobic amino acid side chain analogs using different water models. <i>Journal of Chemical Physics</i> , 2017, 146, 225104.	3.0	18
32	Dynamics of Water in the Hydration Layer of a Partially Unfolded Structure of the Protein HP-36. <i>Journal of Physical Chemistry B</i> , 2008, 112, 6500-6507.	2.6	16
33	Comparison of hydration behavior and conformational preferences of the Trp-cage mini-protein in different rigid-body water models. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32796-32813.	2.8	16
34	Sensitivity of Protein Glass Transition to the Choice of Water Model. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5643-5655.	5.3	16
35	Operation of Kelvin Effect in the Activities of an Antifreeze Protein: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3079-3087.	2.6	16
36	Microscopic Hydration Properties of the A β 42 Peptide Monomer and the Globular Protein Ubiquitin: A Comparative Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11591-11604.	2.6	15

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37	Effects of Metal Ions on β Peptide Conformations from Molecular Simulation Studies. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2879-2893.	5.4	15
38	Microscopic dynamics of water around unfolded structures of barstar at room temperature. <i>Journal of Chemical Physics</i> , 2015, 142, 055102.	3.0	14
39	Low-Frequency Vibrational Spectrum of Water around Cyclodextrin and Its Methyl-Substituted Derivatives. <i>Langmuir</i> , 2010, 26, 14097-14102.	3.5	13
40	Dynamical crossover of water confined within the amphiphilic nanocores of aggregated amyloid β peptides. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14835-14845.	2.8	13
41	Correlated Dynamical Crossovers of the Hydration Layer of a Single-Stranded DNA Oligomer. <i>Journal of Physical Chemistry B</i> , 2014, 118, 413-422.	2.6	12
42	Size-Dependent Conformational Features of β Protofilaments from Molecular Simulation Studies. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2378-2392.	5.4	12
43	Conformational fluctuations of a protein-DNA complex and the structure and ordering of water around it. <i>Journal of Chemical Physics</i> , 2011, 135, 245104.	3.0	11
44	Dynamics of water around the complex structures formed between the KH domains of far upstream element binding protein and single-stranded DNA molecules. <i>Journal of Chemical Physics</i> , 2015, 143, 045106.	3.0	11
45	Role of Polar and Nonpolar Groups in the Activity of Antifreeze Proteins: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9389-9398.	2.6	11
46	Monte Carlo and molecular dynamics simulation of argon clusters and n-alkanes in the confined regions of zeolites. <i>Bulletin of Materials Science</i> , 1997, 20, 845-878.	1.7	10
47	Effects of protein conformational motions in the native form and non-uniform distribution of electrostatic interaction sites on interfacial water. <i>Chemical Physics</i> , 2013, 420, 35-43.	1.9	10
48	Vibrational spectrum of water confined in and around cyclodextrins. <i>Chemical Physics Letters</i> , 2011, 509, 181-185.	2.6	9
49	Intermolecular Dynamics of Water: Suitability of Reactive Interatomic Potential. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6529-6535.	2.6	9
50	Secondary Structure Specific Entropy Change of a Partially Unfolded Protein Molecule. <i>Langmuir</i> , 2010, 26, 9911-9916.	3.5	8
51	Correlated Conformational Motions of the KH Domains of Far Upstream Element Binding Protein Complexed with Single-Stranded DNA Oligomers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10998-11009.	2.6	7
52	Understanding the microscopic origin behind heterogeneous properties of water confined in and around β protofilaments. <i>Journal of Chemical Physics</i> , 2018, 149, 065101.	3.0	7
53	Thermal unfolding of barstar and the properties of interfacial water around the unfolded forms. <i>Journal of Chemical Physics</i> , 2013, 139, 235101.	3.0	6
54	Hydration Behavior along the Folding Pathways of Trpzip4, Trpzip5 and Trpzip6. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1560-1572.	2.6	6

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55	Contrasting Effects of Ionic Liquids of Varying Degree of Hydrophilicity on the Conformational and Interfacial Properties of a Globular Protein. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9441-9453.	2.6	6
56	Dynamic Heterogeneity at the Interface of an Intrinsically Disordered Peptide. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1942-1955.	5.4	6
57	In silico studies of the early stages of aggregation of A β_{42} peptides. <i>Journal of Chemical Sciences</i> , 2017, 129, 899-909.	1.5	5
58	The sensitivity of folding free energy landscapes of trpzips to mutations in the hydrophobic core. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22813-22825.	2.8	5
59	Importance of Solvent in Guiding the Conformational Properties of an Intrinsically Disordered Peptide. <i>Langmuir</i> , 2021, 37, 14429-14442.	3.5	5
60	Thermodynamics of complex structures formed between single-stranded DNA oligomers and the KH domains of the far upstream element binding protein. <i>Journal of Chemical Physics</i> , 2016, 144, 205105.	3.0	4
61	Effects of protein-DNA complex formation on the intermolecular vibrational density of states of interfacial water. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7780-7788.	2.8	4
62	Flexibility of the Binding Regions of a Protein-DNA Complex and the Structure and Ordering of Interfacial Water. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4427-4437.	5.4	4
63	Exploring Heterogeneous Dynamical Environment around an Ensemble of β_{42} Peptide Monomer Conformations. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3453-3462.	5.4	4
64	Effect of temperature on the low-frequency vibrational spectrum and relative structuring of hydration water around a single-stranded DNA. <i>Journal of Chemical Physics</i> , 2015, 142, 015101.	3.0	3
65	Microscopic understanding of the conformational features of a protein-DNA complex. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32459-32472.	2.8	3
66	Heterogeneous Dynamical Environment at the Interface of a Protein-DNA Complex. <i>Langmuir</i> , 2020, 36, 4567-4581.	3.5	3
67	Effect of aggregated β -protofilaments on intermolecular vibrational spectrum of confined water. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.	1.5	2
68	Effect of unfolding on the thickness of the hydration layer of a protein. <i>Indian Journal of Physics</i> , 2009, 83, 49-64.	1.8	1