Shekhar Garde

List of Publications by Year
in descending order

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90	7,454	47006	51608
papers	citations	47	86
		h-index	g-index

92	92	92	6577
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Osmotic water transport through carbon nanotube membranes. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 10175-10180.	7.1	816
2	Water in Nonpolar Confinement: From Nanotubes to Proteins and Beyond. Annual Review of Physical Chemistry, 2008, 59, 713-740.	10.8	624
3	Characterizing hydrophobicity of interfaces by using cavity formation, solute binding, and water correlations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15119-15124.	7.1	309
4	Hydrophobic hydration from small to large lengthscales: Understanding and manipulating the crossover. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 9475-9480.	7.1	268
5	How Wetting and Adhesion Affect Thermal Conductance of a Range of Hydrophobic to Hydrophilic Aqueous Interfaces. Physical Review Letters, 2009, 102, 156101.	7.8	251
6	Origin of Entropy Convergence in Hydrophobic Hydration and Protein Folding. Physical Review Letters, 1996, 77, 4966-4968.	7.8	246
7	Hydration of Enzyme in Nonaqueous Media Is Consistent with Solvent Dependence of Its Activity. Biophysical Journal, 2004, 87, 812-821.	0.5	219
8	Hydrophobicity of Proteins and Interfaces: Insights from Density Fluctuations. Annual Review of Chemical and Biomolecular Engineering, 2011, 2, 147-171.	6.8	192
9	Mapping hydrophobicity at the nanoscale: Applications to heterogeneous surfaces and proteins. Faraday Discussions, 2010, 146, 353.	3.2	191
10	Sitting at the Edge: How Biomolecules use Hydrophobicity to Tune Their Interactions and Function. Journal of Physical Chemistry B, 2012, 116, 2498-2503.	2.6	191
11	Salting-In and Salting-Out of Hydrophobic Solutes in Aqueous Salt Solutions. Journal of Physical Chemistry B, 2001, 105, 6380-6386.	2.6	163
12	Quantifying Water Density Fluctuations and Compressibility of Hydration Shells of Hydrophobic Solutes and Proteins. Physical Review Letters, 2009, 103, 037803.	7.8	152
13	Molecular Dynamics Simulations of Pressure Effects on Hydrophobic Interactions. Journal of the American Chemical Society, 2001, 123, 10997-11003.	13.7	146
14	Size dependent ion hydration, its asymmetry, and convergence to macroscopic behavior. Journal of Chemical Physics, 2004, 120, 4457-4466.	3.0	140
15	Extended surfaces modulate hydrophobic interactions of neighboring solutes. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 17678-17683.	7.1	140
16	Osmolyte Trimethylamine-N-Oxide Does Not Affect the Strength of Hydrophobic Interactions: Origin of Osmolyte Compatibility. Biophysical Journal, 2005, 89, 858-866.	0.5	138
17	Cavity Expulsion and Weak Dewetting of Hydrophobic Solutes in Water. Physical Review Letters, 1998, 80, 4193-4196.	7.8	126
18	On the Salt-Induced Stabilization of Pair and Many-body Hydrophobic Interactions. Journal of Physical Chemistry B, 2005, 109, 642-651.	2.6	120

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19	Effects of lengthscales and attractions on the collapse of hydrophobic polymers in water. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 733-738.	7.1	113
20	Temperature dependence of the solubility of non-polar gases in water. Biophysical Chemistry, 1999, 78, 21-32.	2.8	98
21	Conformational Diffusion and Helix Formation Kinetics. Physical Review Letters, 2000, 85, 2637-2640.	7.8	96
22	Role of Backbone Hydration and Salt-Bridge Formation in Stability of Î±-Helix in Solution. Biophysical Journal, 2003, 85, 3187-3193.	0.5	95
23	Pathways to dewetting in hydrophobic confinement. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 8181-8186.	7.1	95
24	Direct determination of phase behavior of square-well fluids. Journal of Chemical Physics, 2005, 123, 174505.	3.0	94
25	Thermal Resistance of Nanoscopic Liquidâ^'Liquid Interfaces:â€‰ Dependence on Chemistry and Molecular Architecture. Nano Letters, 2005, 5, 2225-2231.	9.1	93
26	Quantifying Density Fluctuations in Volumes of All Shapes and Sizes Using Indirect Umbrella Sampling. Journal of Statistical Physics, 2011, 145, 265-275.	1.2	90
27	Enthalpy and entropy contributions to the pressure dependence of hydrophobic interactions. Journal of Chemical Physics, 2002, 116, 2480-2486.	3.0	81
28	Hydrophobicity of proteins and nanostructured solutes is governed by topographical and chemical context. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13345-13350.	7.1	81
29	How Chemistry, Nanoscale Roughness, and the Direction of Heat Flow Affect Thermal Conductance of Solidâ€“Water Interfaces. Industrial & Engineering Chemistry Research, 2012, 51, 1767-1773.	3.7	78
30	Molecular structure and hydrophobic solvation thermodynamics at an octaneâ€“water interface. Journal of Chemical Physics, 2003, 119, 9199-9206.	3.0	77
31	Efficient affinity maturation of antibody variable domains requires co-selection of compensatory mutations to maintain thermodynamic stability. Scientific Reports, 2017, 7, 45259.	3.3	77
32	Efficient Method To Characterize the Context-Dependent Hydrophobicity of Proteins. Journal of Physical Chemistry B, 2014, 118, 1564-1573.	2.6	75
33	How Surface Wettability Affects the Binding, Folding, and Dynamics of Hydrophobic Polymers at Interfaces. Langmuir, 2009, 25, 13092-13099.	3.5	69
34	Water-mediated ionâ€“ion interactions are enhanced at the water vaporâ€“liquid interface. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 8729-8734.	7.1	69
35	Unfolding of Hydrophobic Polymers in Guanidinium Chloride Solutions. Journal of Physical Chemistry B, 2010, 114, 2246-2254.	2.6	66
36	Temperature dependence of hydrophobic hydration and entropy convergence in an isotropic model of water. Journal of Chemical Physics, 2001, 115, 977-982.	3.0	63

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37	Modeling the selective partitioning of cations into negatively charged nanopores in water. Journal of Chemical Physics, 2007, 126, 084706.	3.0	63
38	Unraveling the hydrophobic effect, one molecule at a time. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16491-16492.	7.1	61
39	Mesoscale model of polymer melt structure: Self-consistent mapping of molecular correlations to coarse-grained potentials. Journal of Chemical Physics, 2005, 122, 104908.	3.0	60
40	Free energy of hydration of a molecular ionic solute: Tetramethylammonium ion. Journal of Chemical Physics, 1998, 108, 1552-1561.	3.0	59
41	Enthalpyâ^'Entropy Contributions to Salt and Osmolyte Effects on Molecular-Scale Hydrophobic Hydration and Interactions. Journal of Physical Chemistry B, 2008, 112, 5661-5670.	2.6	57
42	Molecular dynamics simulation of C8E5micelle in explicit water: structure and hydrophobic solvation thermodynamics. Molecular Physics, 2002, 100, 2299-2306.	1.7	54
43	Water-Mediated Three-Particle Interactions between Hydrophobic Solutes:Â Size, Pressure, and Salt Effects. Journal of Physical Chemistry B, 2003, 107, 612-617.	2.6	54
44	Methane Partitioning and Transport in Hydrated Carbon Nanotubes. Journal of Physical Chemistry B, 2004, 108, 544-549.	2.6	52
45	Arginine mutations in antibody complementarity-determining regions display context-dependent affinity/specificity trade-offs. Journal of Biological Chemistry, 2017, 292, 16638-16652.	3.4	51
46	Hydrophobic hydration: Inhomogeneous water structure near nonpolar molecular solutes. Physical Review E, 1996, 53, R4310-R4313.	2.1	50
47	Evaluation of selectivity changes in HIC systems using a preferential interaction based analysis. Biotechnology and Bioengineering, 2004, 87, 354-363.	3.3	48
48	Do Inverse Monte Carlo Algorithms Yield Thermodynamically Consistent Interaction Potentials?. Industrial & Engineering Chemistry Research, 2006, 45, 5614-5618.	3.7	48
49	The hydrophobic effect. Current Opinion in Colloid and Interface Science, 1996, 1, 376-383.	7.4	46
50	Reply to Comment on â€œElectrostatic Potentials and Free Energies of Solvation of Polar and Charged Moleculesâ€• Journal of Physical Chemistry B, 1998, 102, 3841-3843.	2.6	44
51	Conformational Equilibria of Alkanes in Aqueous Solution: Relationship to Water Structure Near Hydrophobic Solutes. Biophysical Journal, 1999, 77, 645-654.	0.5	43
52	Mechanism for Intein C-Terminal Cleavage: A Proposal from Quantum Mechanical Calculations. Biophysical Journal, 2007, 92, 847-853.	0.5	42
53	Studying pressure denaturation of a protein by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1641-1651.	2.6	42
54	Molecular Simulations of Multimodal Ligandâ€“Protein Binding: Elucidation of Binding Sites and Correlation with Experiments. Journal of Physical Chemistry B, 2011, 115, 13320-13327.	2.6	41

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55	Hydrophobic interactions in context. Nature, 2015, 517, 277-279.	27.8	39
56	Hydrophobic interactions: conformational equilibria and the association of non-polar molecules in water. Faraday Discussions, 1996, 103, 125.	3.2	37
57	Tail Ordering Due to Headgroup Hydrogen Bonding Interactions in Surfactant Monolayers at the Waterâ^'Oil Interface. Journal of Physical Chemistry B, 2006, 110, 19093-19096.	2.6	37
58	How Interfaces Affect Hydrophobically Driven Polymer Folding. Journal of Physical Chemistry B, 2009, 113, 4093-4101.	2.6	35
59	On the Thermodynamics and Kinetics of Hydrophobic Interactions at Interfaces. Journal of Physical Chemistry B, 2013, 117, 10261-10270.	2.6	34
60	Trimethylamine N-Oxide (TMAO) and tert-Butyl Alcohol (TBA) at Hydrophobic Interfaces: Insights from Molecular Dynamics Simulations. Langmuir, 2013, 29, 8017-8024.	3.5	31
61	Role of Arginine in Mediating Proteinâ€“Carbon Nanotube Interactions. Langmuir, 2015, 31, 1683-1692.	3.5	30
62	Structure, Stability, and Rupture of Free and Supported Liquid Films and Assemblies in Molecular Simulations. Industrial & Engineering Chemistry Research, 2008, 47, 3582-3590.	3.7	28
63	Configuration of PKCÎ±-C2 Domain Bound to Mixed SOPC/SOPS Lipid Monolayers. Biophysical Journal, 2009, 97, 2794-2802.	0.5	27
64	Self-Assembly of TMAO at Hydrophobic Interfaces and Its Effect on Protein Adsorption: Insights from Experiments and Simulations. Langmuir, 2010, 26, 9695-9702.	3.5	26
65	Helix propensities of short peptides: Molecular dynamics versus bioinformatics. Proteins: Structure, Function and Bioinformatics, 2003, 50, 552-562.	2.6	25
66	Single Molecule Force Spectroscopy and Molecular Dynamics Simulations as a Combined Platform for Probing Protein Face-Specific Binding. Langmuir, 2017, 33, 10851-10860.	3.5	24
67	Attractions, Water Structure, and Thermodynamics of Hydrophobic Polymer Collapse. Journal of Physical Chemistry B, 2008, 112, 13193-13196.	2.6	23
68	Interactions of Multimodal Ligands with Proteins: Insights into Selectivity Using Molecular Dynamics Simulations. Langmuir, 2015, 31, 7512-7523.	3.5	21
69	The entropy of hydration of simple hydrophobic solutes. Biophysical Chemistry, 1994, 51, 349-357.	2.8	20
70	Application of a Spherical Harmonics Expansion Approach for Calculating Ligand Density Distributions around Proteins. Journal of Physical Chemistry B, 2014, 118, 13066-13076.	2.6	18
71	Quantifying the protein core flexibility through analysis of cavity formation. Journal of Chemical Physics, 2006, 124, 074704.	3.0	16
72	Hydration Dynamics at Femtosecond Time Scales and Angstrom Length Scales from Inelastic X-Ray Scattering. Physical Review Letters, 2009, 103, 237402.	7.8	16

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73	Designing Heteropolymers To Fold into Unique Structures via Water-Mediated Interactions. Journal of Physical Chemistry B, 2010, 114, 13282-13288.	2.6	13
74	Microscopic density fluctuations and solvation in polymeric fluids. Journal of Chemical Physics, 2000, 112, 1574-1578.	3.0	10
75	Mechanistic studies of displacerâ€“protein binding in chemically selective displacement systems using NMR and MD simulations. Biotechnology and Bioengineering, 2009, 102, 1428-1437.	3.3	10
76	Pressure dependence of the compressibility of a micelle and a protein: insights from cavity formation analysis. Molecular Physics, 2007, 105, 189-199.	1.7	9
77	Lengthscale-Dependent Solvation and Density Fluctuations in n-Octane. Journal of Physical Chemistry B, 2015, 119, 9287-9294.	2.6	9
78	Formation of Ligand Clusters on Multimodal Chromatographic Surfaces. Langmuir, 2019, 35, 16770-16779.	3.5	9
79	Water at functional interfaces. MRS Bulletin, 2014, 39, 1051-1053.	3.5	8
80	Effect of guanidine and arginine on proteinâ€“ligand interactions in multimodal cationâ€exchange chromatography. Biotechnology Progress, 2017, 33, 435-447.	2.6	8
81	Conformational Equilibria of Multimodal Chromatography Ligands in Water and Bound to Protein Surfaces. Journal of Physical Chemistry B, 2019, 123, 4833-4843.	2.6	6
82	Detailed molecular simulations to investigate multicomponent diffusion models. AICHE Journal, 2006, 52, 1304-1307.	3.6	5
83	Bridging Gaussian Density Fluctuations from Microscopic to Macroscopic Volumes: Applications to Non-Polar Solute Hydration Thermodynamics. Journal of Physical Chemistry B, 2021, 125, 8152-8164.	2.6	5
84	The Role of Ligandâ€“Ligand Interactions in Multimodal Ligand Conformational Equilibria and Surface Pattern Formation. Langmuir, 2020, 36, 9054-9063.	3.5	4
85	Sticky when dry. Nature Chemistry, 2020, 12, 587-588.	13.6	4
86	Structure and Dynamics of Single Hydrophobic/Ionic Heteropolymers at the Vaporâ€“Liquid Interface of Water. Langmuir, 2014, 30, 4654-4661.	3.5	3
87	Understanding n-Octane Behavior near Graphene with Scaled Solventâ€“Solute Attractions. Journal of Physical Chemistry B, 2016, 120, 2033-2042.	2.6	2
88	Binding, Structure, and Dynamics of Hydrophobic Polymers near Patterned Self-Assembled Monolayer Surfaces. Langmuir, 2014, 30, 14204-14211.	3.5	1
89	The Effects of Ligand Structure on Protein-Multimodal Ligand Interactions. Biophysical Journal, 2019, 116, 477a.	0.5	1
90	Molecularium Explores the World of Materials. MRS Bulletin, 2005, 30, 132-133.	3.5	0