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	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
2	The Role of Ligandâ€“Ligand Interactions in Multimodal Ligand Conformational Equilibria and Surface Pattern Formation. Langmuir, 2020, 36, 9054-9063.	3.5	4
3	Sticky when dry. Nature Chemistry, 2020, 12, 587-588.	13.6	4
4	Formation of Ligand Clusters on Multimodal Chromatographic Surfaces. Langmuir, 2019, 35, 16770-16779.	3.5	9
5	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
6	The Effects of Ligand Structure on Protein-Multimodal Ligand Interactions. Biophysical Journal, 2019, 116, 477a.	0.5	1
7	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
8	Effect of guanidine and arginine on proteinâ€“ligand interactions in multimodal cationâ€exchange chromatography. Biotechnology Progress, 2017, 33, 435-447.	2.6	8
9	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
10	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
11	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
12	Understanding n-Octane Behavior near Graphene with Scaled Solventâ€“Solute Attractions. Journal of Physical Chemistry B, 2016, 120, 2033-2042.	2.6	2
13	Role of Arginine in Mediating Proteinâ€“Carbon Nanotube Interactions. Langmuir, 2015, 31, 1683-1692.	3.5	30
14	Hydrophobic interactions in context. Nature, 2015, 517, 277-279.	27.8	39
15	Interactions of Multimodal Ligands with Proteins: Insights into Selectivity Using Molecular Dynamics Simulations. Langmuir, 2015, 31, 7512-7523.	3.5	21
16	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
17	Lengthscale-Dependent Solvation and Density Fluctuations in n-Octane. Journal of Physical Chemistry B, 2015, 119, 9287-9294.	2.6	9
18	Binding, Structure, and Dynamics of Hydrophobic Polymers near Patterned Self-Assembled Monolayer Surfaces. Langmuir, 2014, 30, 14204-14211.	3.5	1

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19	Water at functional interfaces. MRS Bulletin, 2014, 39, 1051-1053.	3.5	8
20	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
21	Structure and Dynamics of Single Hydrophobic/Ionic Heteropolymers at the Vaporâ€“Liquid Interface of Water. Langmuir, 2014, 30, 4654-4661.	3.5	3
22	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
23	Efficient Method To Characterize the Context-Dependent Hydrophobicity of Proteins. Journal of Physical Chemistry B, 2014, 118, 1564-1573.	2.6	75
24	On the Thermodynamics and Kinetics of Hydrophobic Interactions at Interfaces. Journal of Physical Chemistry B, 2013, 117, 10261-10270.	2.6	34
25	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
26	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
27	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
28	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
29	Hydrophobicity of Proteins and Interfaces: Insights from Density Fluctuations. Annual Review of Chemical and Biomolecular Engineering, 2011, 2, 147-171.	6.8	192
30	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
31	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
32	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
33	Studying pressure denaturation of a protein by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1641-1651.	2.6	42
34	Unfolding of Hydrophobic Polymers in Guanidinium Chloride Solutions. Journal of Physical Chemistry B, 2010, 114, 2246-2254.	2.6	66
35	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
36	Designing Heteropolymers To Fold into Unique Structures via Water-Mediated Interactions. Journal of Physical Chemistry B, 2010, 114, 13282-13288.	2.6	13

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37	Mapping hydrophobicity at the nanoscale: Applications to heterogeneous surfaces and proteins. Faraday Discussions, 2010, 146, 353.	3.2	191
38	Hydration Dynamics at Femtosecond Time Scales and Angstrom Length Scales from Inelastic X-Ray Scattering. Physical Review Letters, 2009, 103, 237402.	7.8	16
39	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
40	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
41	How Surface Wettability Affects the Binding, Folding, and Dynamics of Hydrophobic Polymers at Interfaces. Langmuir, 2009, 25, 13092-13099.	3.5	69
42	Configuration of PKCÎ±-C2 Domain Bound to Mixed SOPC/SOPS Lipid Monolayers. Biophysical Journal, 2009, 97, 2794-2802.	0.5	27
43	How Interfaces Affect Hydrophobically Driven Polymer Folding. Journal of Physical Chemistry B, 2009, 113, 4093-4101.	2.6	35
44	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
45	Quantifying Water Density Fluctuations and Compressibility of Hydration Shells of Hydrophobic Solutes and Proteins. Physical Review Letters, 2009, 103, 037803.	7.8	152
46	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
47	Water in Nonpolar Confinement: From Nanotubes to Proteins and Beyond. Annual Review of Physical Chemistry, 2008, 59, 713-740.	10.8	624
48	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
49	Attractions, Water Structure, and Thermodynamics of Hydrophobic Polymer Collapse. Journal of Physical Chemistry B, 2008, 112, 13193-13196.	2.6	23
50	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
51	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
52	Modeling the selective partitioning of cations into negatively charged nanopores in water. Journal of Chemical Physics, 2007, 126, 084706.	3.0	63
53	Mechanism for Intein C-Terminal Cleavage: A Proposal from Quantum Mechanical Calculations. Biophysical Journal, 2007, 92, 847-853.	0.5	42
54	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

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55	Do Inverse Monte Carlo Algorithms Yield Thermodynamically Consistent Interaction Potentials?. Industrial & Engineering Chemistry Research, 2006, 45, 5614-5618.	3.7	48
56	Detailed molecular simulations to investigate multicomponent diffusion models. AICHE Journal, 2006, 52, 1304-1307.	3.6	5
57	Quantifying the protein core flexibility through analysis of cavity formation. Journal of Chemical Physics, 2006, 124, 074704.	3.0	16
58	Molecularium Explores the World of Materials. MRS Bulletin, 2005, 30, 132-133.	3.5	0
59	Direct determination of phase behavior of square-well fluids. Journal of Chemical Physics, 2005, 123, 174505.	3.0	94
60	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
61	On the Salt-Induced Stabilization of Pair and Many-body Hydrophobic Interactions. Journal of Physical Chemistry B, 2005, 109, 642-651.	2.6	120
62	Thermal Resistance of Nanoscopic Liquidâ"Liquid Interfaces:â€‰ Dependence on Chemistry and Molecular Architecture. Nano Letters, 2005, 5, 2225-2231.	9.1	93
63	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
64	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
65	Evaluation of selectivity changes in HIC systems using a preferential interaction based analysis. Biotechnology and Bioengineering, 2004, 87, 354-363.	3.3	48
66	Methane Partitioning and Transport in Hydrated Carbon Nanotubes. Journal of Physical Chemistry B, 2004, 108, 544-549.	2.6	52
67	Size dependent ion hydration, its asymmetry, and convergence to macroscopic behavior. Journal of Chemical Physics, 2004, 120, 4457-4466.	3.0	140
68	Hydration of Enzyme in Nonaqueous Media Is Consistent with Solvent Dependence of Its Activity. Biophysical Journal, 2004, 87, 812-821.	0.5	219
69	Helix propensities of short peptides: Molecular dynamics versus bioinformatics. Proteins: Structure, Function and Bioinformatics, 2003, 50, 552-562.	2.6	25
70	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
71	Role of Backbone Hydration and Salt-Bridge Formation in Stability of Î±-Helix in Solution. Biophysical Journal, 2003, 85, 3187-3193.	0.5	95
72	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

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73	Molecular structure and hydrophobic solvation thermodynamics at an octaneâ€“water interface. Journal of Chemical Physics, 2003, 119, 9199-9206.	3.0	77
74	Enthalpy and entropy contributions to the pressure dependence of hydrophobic interactions. Journal of Chemical Physics, 2002, 116, 2480-2486.	3.0	81
75	Molecular dynamics simulation of C8E5micelle in explicit water: structure and hydrophobic solvation thermodynamics. Molecular Physics, 2002, 100, 2299-2306.	1.7	54
76	Salting-In and Salting-Out of Hydrophobic Solutes in Aqueous Salt Solutions. Journal of Physical Chemistry B, 2001, 105, 6380-6386.	2.6	163
77	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
78	Molecular Dynamics Simulations of Pressure Effects on Hydrophobic Interactions. Journal of the American Chemical Society, 2001, 123, 10997-11003.	13.7	146
79	Microscopic density fluctuations and solvation in polymeric fluids. Journal of Chemical Physics, 2000, 112, 1574-1578.	3.0	10
80	Conformational Diffusion and Helix Formation Kinetics. Physical Review Letters, 2000, 85, 2637-2640.	7.8	96
81	Temperature dependence of the solubility of non-polar gases in water. Biophysical Chemistry, 1999, 78, 21-32.	2.8	98
82	Conformational Equilibria of Alkanes in Aqueous Solution: Relationship to Water Structure Near Hydrophobic Solutes. Biophysical Journal, 1999, 77, 645-654.	0.5	43
83	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
84	Free energy of hydration of a molecular ionic solute: Tetramethylammonium ion. Journal of Chemical Physics, 1998, 108, 1552-1561.	3.0	59
85	Cavity Expulsion and Weak Dewetting of Hydrophobic Solutes in Water. Physical Review Letters, 1998, 80, 4193-4196.	7.8	126
86	Origin of Entropy Convergence in Hydrophobic Hydration and Protein Folding. Physical Review Letters, 1996, 77, 4966-4968.	7.8	246
87	Hydrophobic interactions: conformational equilibria and the association of non-polar molecules in water. Faraday Discussions, 1996, 103, 125.	3.2	37
88	The hydrophobic effect. Current Opinion in Colloid and Interface Science, 1996, 1, 376-383.	7.4	46
89	Hydrophobic hydration: Inhomogeneous water structure near nonpolar molecular solutes. Physical Review E, 1996, 53, R4310-R4313.	2.1	50
90	The entropy of hydration of simple hydrophobic solutes. Biophysical Chemistry, 1994, 51, 349-357.	2.8	20