Joachim Dzubiella

List of Publications by Year
in descending order

123	5,714	101543	82547
papers	citations	36 h-index	72 g-index

124	124	124	7615
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Catalysis by metallic nanoparticles in aqueous solution: model reactions. Chemical Society Reviews, 2012, 41, 5577.	38.1	966
2	Protein Interactions with Polymer Coatings and Biomaterials. Angewandte Chemie - International Edition, 2014, 53, 8004-8031.	13.8	614
3	Beyond the Hofmeister Series: Ion-Specific Effects on Proteins and Their Biological Functions. Journal of Physical Chemistry B, 2017, 121, 1997-2014.	2.6	466
4	Thermosensitive Auâ€PNIPA Yolkâ€“Shell Nanoparticles with Tunable Selectivity for Catalysis. Angewandte Chemie - International Edition, 2012, 51, 2229-2233.	13.8	350
5	Ion Specificity at the Peptide Bond: Molecular Dynamics Simulations of N-Methylacetamide in Aqueous Salt Solutions. Journal of Physical Chemistry B, 2010, 114, 1213-1220.	2.6	107
6	Coreâ€“shell microgels as â€œsmartâ€•carriers for enzymes. Soft Matter, 2012, 8, 1428-1436.	2.7	103
7	Structure-thermodynamics relation of electrolyte solutions. Journal of Chemical Physics, 2009, 130, 134507.	3.0	99
8	Adsorption of proteins to functional polymeric nanoparticles. Polymer, 2013, 54, 2835-2849.	3.8	94
9	Thermodynamic Description of Hofmeister Effects on the LCST of Thermosensitive Polymers. Journal of Physical Chemistry B, 2014, 118, 10979-10988.	2.6	93
10	Salt-Specific Stability and Denaturation of a Short Salt-Bridge-Forming Î±-Helix. Journal of the American Chemical Society, 2008, 130, 14000-14007.	13.7	89
11	Rationalizing Polymer Swelling and Collapse under Attractive Cosolvent Conditions. Macromolecules, 2013, 46, 1231-1238.	4.8	88
12	Solvent fluctuations in hydrophobic cavityâ€“ligand binding kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1197-1202.	7.1	86
13	Application of the level-set method to the implicit solvation of nonpolar molecules. Journal of Chemical Physics, 2007, 127, 084503.	3.0	81
14	Molecular simulations of electrolyte structure and dynamics in lithiumâ€“sulfur battery solvents. Journal of Power Sources, 2018, 373, 70-78.	7.8	79
15	Protein Sorption to Charged Microgels: Characterizing Binding Isotherms and Driving Forces. Langmuir, 2012, 28, 14373-14385.	3.5	76
16	Guanidinium can both Cause and Prevent the Hydrophobic Collapse of Biomacromolecules. Journal of the American Chemical Society, 2017, 139, 863-870.	13.7	76
17	Confined Water Determines Transport Properties of Guest Molecules in Narrow Pores. ACS Nano, 2016, 10, 7646-7656.	14.6	66
18	Interaction of human serum albumin with short polyelectrolytes: a study by calorimetry and computer simulations. Soft Matter, 2015, 11, 4630-4639.	2.7	64

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19	Competitive adsorption of multiple proteins to nanoparticles: the Vroman effect revisited. Molecular Physics, 2018, 116, 3154-3163.	1.7	58
20	Catalyzed Bimolecular Reactions in Responsive Nanoreactors. ACS Catalysis, 2017, 7, 5604-5611.	11.2	53
21	Interaction of Proteins with Polyelectrolytes: Comparison of Theory to Experiment. Langmuir, 2019, 35, 5373-5391.	3.5	51
22	Thermodynamic Description of the LCST of Charged Thermoresponsive Copolymers. Macromolecules, 2014, 47, 2096-2102.	4.8	47
23	Like-charged protein-polyelectrolyte complexation driven by charge patches. Journal of Chemical Physics, 2015, 143, 064905.	3.0	47
24	Effects of Hofmeister Ions on the Î±-Helical Structure of Proteins. Biophysical Journal, 2012, 102, 907-915.	0.5	46
25	Thermosensitive Cu₂Oâ€“PNIPAM coreâ€“shell nanoreactors with tunable photocatalytic activity. Journal of Materials Chemistry A, 2016, 4, 9677-9684.	10.3	46
26	Variational Implicit Solvation with Poissonâ€“Boltzmann Theory. Journal of Chemical Theory and Computation, 2014, 10, 1454-1467.	5.3	45
27	Coupling the Level-Set Method with Molecular Mechanics for Variational Implicit Solvation of Nonpolar Molecules. Journal of Chemical Theory and Computation, 2009, 5, 257-266.	5.3	44
28	Ion-specific counterion condensation on charged peptides: Poissonâ€“Boltzmann vs. atomistic simulations. Soft Matter, 2012, 8, 9338.	2.7	44
29	Interaction of Charged Patchy Protein Models with Like-Charged Polyelectrolyte Brushes. Langmuir, 2017, 33, 417-427.	3.5	44
30	Ion-Specific Excluded-Volume Correlations and Solvation Forces. Physical Review Letters, 2010, 104, 097802.	7.8	42
31	Catalysis by Metallic Nanoparticles in Solution: Thermosensitive Microgels as Nanoreactors. Zeitschrift Fur Physikalische Chemie, 2018, 232, 773-803.	2.8	42
32	Interfaces and hydrophobic interactions in receptor-ligand systems: A level-set variational implicit solvent approach. Journal of Chemical Physics, 2009, 131, 144102.	3.0	40
33	Sequence-Specific Size, Structure, and Stability of Tight Protein Knots. Biophysical Journal, 2009, 96, 831-839.	0.5	40
34	Counterion-Release Entropy Governs the Inhibition of Serum Proteins by Polyelectrolyte Drugs. Biomacromolecules, 2018, 19, 409-416.	5.4	39
35	Charged patchy particle models in explicit salt: Ion distributions, electrostatic potentials, and effective interactions. Journal of Chemical Physics, 2015, 143, 064904.	3.0	38
36	Electrolytes in a nanometer slab-confinement: Ion-specific structure and solvation forces. Journal of Chemical Physics, 2010, 133, 164511.	3.0	37

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37	Dynamic density functional theory of protein adsorption on polymer-coated nanoparticles. Soft Matter, 2014, 10, 7932-7945.	2.7	37
38	Theory of Solvation-Controlled Reactions in Stimuli-Responsive Nanoreactors. Journal of Physical Chemistry C, 2015, 119, 15723-15730.	3.1	37
39	Structural and Transport Properties of Li/S Battery Electrolytes: Role of the Polysulfide Species. Journal of Physical Chemistry C, 2019, 123, 10167-10177.	3.1	35
40	Correlation Length in Concentrated Electrolytes: Insights from All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 1778-1786.	2.6	34
41	Level-Set Variational Implicit-Solvent Modeling of Biomolecules with the Coulomb-Field Approximation. Journal of Chemical Theory and Computation, 2012, 8, 386-397.	5.3	33
42	Selective solute adsorption and partitioning around single PNIPAM chains. Physical Chemistry Chemical Physics, 2017, 19, 5906-5916.	2.8	32
43	Charged Dendrimers Revisited: Effective Charge and Surface Potential of Dendritic Polyglycerol Sulfate. Macromolecules, 2017, 50, 4759-4769.	4.8	32
44	Interaction of human serum albumin with dendritic polyglycerol sulfate: Rationalizing the thermodynamics of binding. Journal of Chemical Physics, 2018, 149, 163324.	3.0	32
45	Chasing Aqueous Biphasic Systems from Simple Salts by Exploring the LiTFSI/LiCl/H₂O Phase Diagram. ACS Central Science, 2019, 5, 640-643.	11.3	31
46	How the Shape and Chemistry of Molecular Penetrants Control Responsive Hydrogel Permeability. ACS Nano, 2021, 15, 614-624.	14.6	30
47	Swelling of ionic microgel particles in the presence of excluded-volume interactions: a density functional approach. Physical Chemistry Chemical Physics, 2016, 18, 5372-5385.	2.8	29
48	Competitive Protein Adsorption to Soft Polymeric Layers: Binary Mixtures and Comparison to Theory. Journal of Physical Chemistry B, 2015, 119, 3250-3258.	2.6	28
49	Selective Molecular Transport in Thermoresponsive Polymer Membranes: Role of Nanoscale Hydration and Fluctuations. Macromolecules, 2018, 51, 4853-4864.	4.8	28
50	Evaluation of Hydration Free Energy by Level-Set Variational Implicit-Solvent Model with Coulomb-Field Approximation. Journal of Chemical Theory and Computation, 2013, 9, 1778-1787.	5.3	27
51	Cosolute Partitioning in Polymer Networks: Effects of Flexibility and Volume Transitions. Macromolecules, 2017, 50, 6227-6237.	4.8	27
52	Tuning the selective permeability of polydisperse polymer networks. Soft Matter, 2020, 16, 8144-8154.	2.7	26
53	Tuning the Permeability of Dense Membranes by Shaping Nanoscale Potentials. Physical Review Letters, 2019, 122, 108001.	7.8	23
54	Ion Specificity in Î±-Helical Folding Kinetics. Journal of Physical Chemistry B, 2010, 114, 13815-13822.	2.6	22

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55	Heterogeneous Hydration of p53/MDM2 Complex. Journal of Chemical Theory and Computation, 2014, 10, 1302-1313.	5.3	22
56	Temperature-Dependent Implicit-Solvent Model of Polyethylene Glycol in Aqueous Solution. Journal of Chemical Theory and Computation, 2017, 13, 6317-6327.	5.3	22
57	Salt-Specific Stability of Short and Charged Alanine-Based Î±-Helices. Journal of Physical Chemistry B, 2009, 113, 16689-16694.	2.6	21
58	Sorption and Spatial Distribution of Protein Globules in Charged Hydrogel Particles. Langmuir, 2017, 33, 4567-4577.	3.5	21
59	Modeling of stimuli-responsive nanoreactors: rational rate control towards the design of colloidal enzymes. Molecular Systems Design and Engineering, 2020, 5, 602-619.	3.4	21
60	Aqueous Nanoclusters Govern Ion Partitioning in Dense Polymer Membranes. ACS Nano, 2019, 13, 11224-11234.	14.6	20
61	Transfer Free Energies and Partitioning of Small Molecules in Collapsed PNIPAM Polymers. Journal of Physical Chemistry B, 2019, 123, 720-728.	2.6	20
62	Growth and Characterization of Molecular Crystals of para-Sexiphenyl by All-Atom Computer Simulations. Crystal Growth and Design, 2014, 14, 3791-3799.	3.0	19
63	Ionic structure around polarizable metal nanoparticles in aqueous electrolytes. Soft Matter, 2018, 14, 4053-4063.	2.7	19
64	Tuning the collapse transition of weakly charged polymers by ion-specific screening and adsorption. Soft Matter, 2018, 14, 9631-9642.	2.7	19
65	Thermodynamics of the Binding of Lysozyme to a Dendritic Polyelectrolyte: Electrostatics Versus Hydration. ACS Omega, 2018, 3, 9086-9095.	3.5	19
66	Nonequilibrium Uptake Kinetics of Molecular Cargo into Hollow Hydrogels Tuned by Electrosteric Interactions. ACS Nano, 2019, 13, 1603-1616.	14.6	19
67	Interface dynamics of microscopic cavities in water. Journal of Chemical Physics, 2007, 126, 194504.	3.0	18
68	LS-VISM: A software package for analysis of biomolecular solvation. Journal of Computational Chemistry, 2015, 36, 1047-1059.	3.3	18
69	Reaction rate of a composite coreâ€“shell nanoreactor with multiple nanocatalysts. Physical Chemistry Chemical Physics, 2016, 18, 20758-20767.	2.8	18
70	Curvature Dependence of Hydrophobic Hydration Dynamics. Physical Review Letters, 2015, 114, 187802.	7.8	17
71	Enhanced Catalytic Activity of Gold@Polydopamine Nanoreactors with Multi-compartment Structure Under NIR Irradiation. Nano-Micro Letters, 2019, 11, 83.	27.0	17
72	Controlling the Microstructure and Phase Behavior of Confined Soft Colloids by Active Interaction Switching. Physical Review Letters, 2020, 125, 078001.	7.8	17

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73	Kinetics of the Reduction of 4-Nitrophenol by Silver Nanoparticles Immobilized in Thermoresponsive Coreâ€“Shell Nanoreactors. Industrial & Engineering Chemistry Research, 2021, 60, 3922-3935.	3.7	17
74	Potential of mean force and transient states in polyelectrolyte pair complexation. Journal of Chemical Physics, 2016, 145, 034901.	3.0	16
75	Ion-Specific Adsorption on Bare Gold (Au) Nanoparticles in Aqueous Solutions: Double-Layer Structure and Surface Potentials. Langmuir, 2020, 36, 13457-13468.	3.5	15
76	Tuning the permeability of regular polymeric networks by the cross-link ratio. Journal of Chemical Physics, 2021, 154, 154902.	3.0	15
77	Cross-linker effect on solute adsorption in swollen thermoresponsive polymer networks. Physical Chemistry Chemical Physics, 2019, 21, 6588-6599.	2.8	14
78	Principles for Tuning Hydrophobic Ligandâ€“Receptor Binding Kinetics. Journal of Chemical Theory and Computation, 2017, 13, 3012-3019.	5.3	13
79	Charge and hydration structure of dendritic polyelectrolytes: molecular simulations of polyglycerol sulphate. Soft Matter, 2018, 14, 4300-4310.	2.7	13
80	Competitive sorption of monovalent and divalent ions by highly charged globular macromolecules. Journal of Chemical Physics, 2020, 153, 044904.	3.0	13
81	Non-equilibrium sedimentation of colloids: confocal microscopy and Brownian dynamics simulations. Journal of Physics Condensed Matter, 2008, 20, 494222.	1.8	12
82	Explicit and implicit modeling of nanobubbles in hydrophobic confinement. Anais Da Academia Brasileira De Ciencias, 2010, 82, 3-12.	0.8	12
83	Molecular Insights into the Ion-Specific Kinetics of Anionic Peptides. Journal of Physical Chemistry B, 2010, 114, 7098-7103.	2.6	12
84	Variational Implicit-Solvent Modeling of Hostâ€“Guest Binding: A Case Study on Cucurbit[7]uril|. Journal of Chemical Theory and Computation, 2013, 9, 4195-4204.	5.3	12
85	Variational implicit-solvent predictions of the dryâ€“wet transition pathways for ligandâ€“receptor binding and unbinding kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14989-14994.	7.1	12
86	Thermal Compaction of Disordered and Elastin-like Polypeptides: A Temperature-Dependent, Sequence-Specific Coarse-Grained Simulation Model. Biomacromolecules, 2020, 21, 3523-3538.	5.4	12
87	Active interaction switching controls the dynamic heterogeneity of soft colloidal dispersions. Soft Matter, 2022, 18, 397-411.	2.7	12
88	Constructing Binderâ€•and Carbon Additiveâ€Free Organosulfur Cathodes Based on Conducting Thiolâ€Polymers through Electropolymerization for Lithiumâ€Sulfur Batteries. ChemSusChem, 2022, 15, .	6.8	12
89	Drastic Swelling of Lipid Oligobilayers by Polyelectrolytes: A Potential Molecular Model for the Internal Structure of Lubricating Films in Mammalian Joints. Langmuir, 2018, 34, 1287-1299.	3.5	11
90	Structure and position-dependent properties of inhomogeneous suspensions of responsive colloids. Physical Review E, 2020, 102, 042602.	2.1	11

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91	Structure and dynamics of responsive colloids with dynamical polydispersity. Journal of Physics Condensed Matter, 2021, 33, 174002.	1.8	11
92	How Interface Geometry Dictates Waterâ€™s Thermodynamic Signature in Hydrophobic Association. Journal of Statistical Physics, 2011, 145, 227-239.	1.2	10
93	Stochastic level-set variational implicit-solvent approach to solute-solvent interfacial fluctuations. Journal of Chemical Physics, 2016, 145, 054114.	3.0	10
94	â€œMartinizingâ€•the Variational Implicit Solvent Method (VISM): Solvation Free Energy for Coarse-Grained Proteins. Journal of Physical Chemistry B, 2017, 121, 6538-6548.	2.6	10
95	Active binary switching of soft colloids: stability and structural properties. Soft Matter, 2021, 17, 7682-7696.	2.7	10
96	Anisotropic Electrostatic Friction of para-Sexiphenyl on the ZnO (101Ì…0) Surface. Journal of Physical Chemistry C, 2014, 118, 26368-26376.	3.1	9
97	Tuning the critical solution temperature of polymers by copolymerization. Journal of Chemical Physics, 2015, 143, 243119.	3.0	9
98	Product interactions and feedback in diffusion-controlled reactions. Journal of Chemical Physics, 2018, 148, 064705.	3.0	9
99	Quantifying entropic barriers in single-molecule surface diffusion. Journal of Chemical Physics, 2020, 153, 164713.	3.0	9
100	Highly Heterogeneous Polarization and Solvation of Gold Nanoparticles in Aqueous Electrolytes. ACS Nano, 2021, 15, 13155-13165.	14.6	9
101	Solvent Fluctuations Induce Non-Markovian Kinetics in Hydrophobic Pocket-Ligand Binding. Journal of Physical Chemistry B, 2016, 120, 8127-8136.	2.6	8
102	Probing the protein corona around charged macromolecules: interpretation of isothermal titration calorimetry by binding models and computer simulations. Colloid and Polymer Science, 2020, 298, 747-759.	2.1	8
103	Combined first-principles statistical mechanics approach to sulfur structure in organic cathode hosts for polymer based lithiumâ€“sulfur (Liâ€“S) batteries. Physical Chemistry Chemical Physics, 2021, 23, 26709-26720.	2.8	8
104	Permeability of Polymer Membranes beyond Linear Response. Macromolecules, 2022, 55, 7327-7339.	4.8	7
105	Ion-Specificity: From Solvation Thermodynamics to Molecular Simulations and Back. , 2009, , 231-265.		6
106	Characterization of step-edge barrier crossing of para-sexiphenyl on the ZnO (101Ì„0) surface. Physical Chemistry Chemical Physics, 2016, 18, 25329-25341.	2.8	6
107	Tailoring the Variational Implicit Solvent Method for New Challenges: Biomolecular Recognition and Assembly. Frontiers in Molecular Biosciences, 2018, 5, 13.	3.5	6
108	Coverage Fluctuations and Correlations in Nanoparticle-Catalyzed Diffusion-Influenced Bimolecular Reactions. Journal of Physical Chemistry C, 2020, 124, 24204-24214.	3.1	6

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109	How the hydroxylation state of the (110)-rutile TiO₂ surface governs its electric double layer properties. Physical Chemistry Chemical Physics, 2021, 23, 14770-14782.	2.8	6
110	Effects of oxidative adsorbates and cluster formation on the electronic structure of nanodiamonds. Journal of Computational Chemistry, 2022, 43, 923-929.	3.3	6
111	Modulating internal transition kinetics of responsive macromolecules by collective crowding. Journal of Chemical Physics, 2021, 155, 244902.	3.0	5
112	Effects of salt on the â€˜dryingâ€™ transition and hydrophobic interaction between nano-sized spherical solutes. Molecular Physics, 2013, 111, 3404-3409.	1.7	4
113	Impact of Polarity on Anisotropic Diffusion of Conjugated Organic Molecules on the (101Ì…0) Zinc Oxide Surface. Journal of Physical Chemistry C, 2019, 123, 6549-6559.	3.1	4
114	Communication: Resonance reaction in diffusion-influenced bimolecular reactions. Journal of Chemical Physics, 2016, 144, 081102.	3.0	3
115	Influence of partial fluorination on growth modes of organic molecules on amorphous silicon dioxide. Physical Review Materials, 2022, 6, .	2.4	3
116	Nanochannels and nanodroplets in polymer membranes controlling ionic transport. Current Opinion in Colloid and Interface Science, 2021, 56, 101501.	7.4	2
117	Toward unveiling structure and property relationships from ionic ordering in Li/S battery electrolytes: Neutron total scattering and molecular dynamics simulations. Energy Storage Materials, 2022, 52, 85-93.	18.0	2
118	Affinity, kinetics, and pathways of anisotropic ligands binding to hydrophobic model pockets. Journal of Chemical Physics, 2018, 149, 094902.	3.0	1
119	Electrostatic Reaction Inhibition in Nanoparticle Catalysis. Langmuir, 2021, 37, 6800-6810.	3.5	1
120	Controlling solvent quality by time: Self-avoiding sprints in nonequilibrium polymerization. Physical Review E, 2021, 104, 034501.	2.1	1
121	Special issue in honor of Matthias Ballauff. Colloid and Polymer Science, 2020, 298, 661-662.	2.1	0
122	Facilitating target search in polymer networks: Effects of target size and mixed one-dimensional and three-dimensional diffusion. Physical Review E, 2021, 103, 032502.	2.1	0
123	Nonequilibrium free energy during polymer chain growth. Journal of Chemical Physics, 2022, 156, 084902.	3.0	0