Joachim Dzubiella

List of Publications by Year
in descending order

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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	Active interaction switching controls the dynamic heterogeneity of soft colloidal dispersions. Soft Matter, 2022, 18, 397-411.	2.7	12
2	Nonequilibrium free energy during polymer chain growth. Journal of Chemical Physics, 2022, 156, 084902.	3.0	0
3	Influence of partial fluorination on growth modes of organic molecules on amorphous silicon dioxide. Physical Review Materials, 2022, 6, .	2.4	3
4	Effects of oxidative adsorbates and cluster formation on the electronic structure of nanodiamonds. Journal of Computational Chemistry, 2022, 43, 923-929.	3.3	6
5	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
6	Permeability of Polymer Membranes beyond Linear Response. Macromolecules, 2022, 55, 7327-7339.	4.8	7
7	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
8	Active binary switching of soft colloids: stability and structural properties. Soft Matter, 2021, 17, 7682-7696.	2.7	10
9	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
10	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
11	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
12	Structure and dynamics of responsive colloids with dynamical polydispersity. Journal of Physics Condensed Matter, 2021, 33, 174002.	1.8	11
13	Tuning the permeability of regular polymeric networks by the cross-link ratio. Journal of Chemical Physics, 2021, 154, 154902.	3.0	15
14	Electrostatic Reaction Inhibition in Nanoparticle Catalysis. Langmuir, 2021, 37, 6800-6810.	3.5	1
15	Highly Heterogeneous Polarization and Solvation of Gold Nanoparticles in Aqueous Electrolytes. ACS Nano, 2021, 15, 13155-13165.	14.6	9
16	Nanochannels and nanodroplets in polymer membranes controlling ionic transport. Current Opinion in Colloid and Interface Science, 2021, 56, 101501.	7.4	2
17	Controlling solvent quality by time: Self-avoiding sprints in nonequilibrium polymerization. Physical Review E, 2021, 104, 034501.	2.1	1
18	How the Shape and Chemistry of Molecular Penetrants Control Responsive Hydrogel Permeability. ACS Nano, 2021, 15, 614-624.	14.6	30

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19	Modulating internal transition kinetics of responsive macromolecules by collective crowding. Journal of Chemical Physics, 2021, 155, 244902.	3.0	5
20	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
21	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
22	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
23	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
24	Competitive sorption of monovalent and divalent ions by highly charged globular macromolecules. Journal of Chemical Physics, 2020, 153, 044904.	3.0	13
25	Controlling the Microstructure and Phase Behavior of Confined Soft Colloids by Active Interaction Switching. Physical Review Letters, 2020, 125, 078001.	7.8	17
26	Coverage Fluctuations and Correlations in Nanoparticle-Catalyzed Diffusion-Influenced Bimolecular Reactions. Journal of Physical Chemistry C, 2020, 124, 24204-24214.	3.1	6
27	Quantifying entropic barriers in single-molecule surface diffusion. Journal of Chemical Physics, 2020, 153, 164713.	3.0	9
28	Tuning the selective permeability of polydisperse polymer networks. Soft Matter, 2020, 16, 8144-8154.	2.7	26
29	Structure and position-dependent properties of inhomogeneous suspensions of responsive colloids. Physical Review E, 2020, 102, 042602.	2.1	11
30	Special issue in honor of Matthias Ballauff. Colloid and Polymer Science, 2020, 298, 661-662.	2.1	0
31	Correlation Length in Concentrated Electrolytes: Insights from All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2020, 124, 1778-1786.	2.6	34
32	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
33	Interaction of Proteins with Polyelectrolytes: Comparison of Theory to Experiment. Langmuir, 2019, 35, 5373-5391.	3.5	51
34	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
35	Enhanced Catalytic Activity of Gold@Polydopamine Nanoreactors with Multi-compartment Structure Under NIR Irradiation. Nano-Micro Letters, 2019, 11, 83.	27.0	17
36	Aqueous Nanoclusters Govern Ion Partitioning in Dense Polymer Membranes. ACS Nano, 2019, 13, 11224-11234.	14.6	20

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37	Tuning the Permeability of Dense Membranes by Shaping Nanoscale Potentials. Physical Review Letters, 2019, 122, 108001.	7.8	23
38	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
39	Cross-linker effect on solute adsorption in swollen thermoresponsive polymer networks. Physical Chemistry Chemical Physics, 2019, 21, 6588-6599.	2.8	14
40	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
41	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
42	Transfer Free Energies and Partitioning of Small Molecules in Collapsed PNIPAM Polymers. Journal of Physical Chemistry B, 2019, 123, 720-728.	2.6	20
43	Nonequilibrium Uptake Kinetics of Molecular Cargo into Hollow Hydrogels Tuned by Electrosteric Interactions. ACS Nano, 2019, 13, 1603-1616.	14.6	19
44	Ionic structure around polarizable metal nanoparticles in aqueous electrolytes. Soft Matter, 2018, 14, 4053-4063.	2.7	19
45	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
46	Counterion-Release Entropy Governs the Inhibition of Serum Proteins by Polyelectrolyte Drugs. Biomacromolecules, 2018, 19, 409-416.	5.4	39
47	Catalysis by Metallic Nanoparticles in Solution: Thermosensitive Microgels as Nanoreactors. Zeitschrift Fur Physikalische Chemie, 2018, 232, 773-803.	2.8	42
48	Molecular simulations of electrolyte structure and dynamics in lithiumâ€“sulfur battery solvents. Journal of Power Sources, 2018, 373, 70-78.	7.8	79
49	Tuning the collapse transition of weakly charged polymers by ion-specific screening and adsorption. Soft Matter, 2018, 14, 9631-9642.	2.7	19
50	Affinity, kinetics, and pathways of anisotropic ligands binding to hydrophobic model pockets. Journal of Chemical Physics, 2018, 149, 094902.	3.0	1
51	Selective Molecular Transport in Thermoresponsive Polymer Membranes: Role of Nanoscale Hydration and Fluctuations. Macromolecules, 2018, 51, 4853-4864.	4.8	28
52	Tailoring the Variational Implicit Solvent Method for New Challenges: Biomolecular Recognition and Assembly. Frontiers in Molecular Biosciences, 2018, 5, 13.	3.5	6
53	Interaction of human serum albumin with dendritic polyglycerol sulfate: Rationalizing the thermodynamics of binding. Journal of Chemical Physics, 2018, 149, 163324.	3.0	32
54	Product interactions and feedback in diffusion-controlled reactions. Journal of Chemical Physics, 2018, 148, 064705.	3.0	9

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55	Charge and hydration structure of dendritic polyelectrolytes: molecular simulations of polyglycerol sulphate. Soft Matter, 2018, 14, 4300-4310.	2.7	13
56	Thermodynamics of the Binding of Lysozyme to a Dendritic Polyelectrolyte: Electrostatics Versus Hydration. ACS Omega, 2018, 3, 9086-9095.	3.5	19
57	Competitive adsorption of multiple proteins to nanoparticles: the Vroman effect revisited. Molecular Physics, 2018, 116, 3154-3163.	1.7	58
58	Selective solute adsorption and partitioning around single PNIPAM chains. Physical Chemistry Chemical Physics, 2017, 19, 5906-5916.	2.8	32
59	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
60	Sorption and Spatial Distribution of Protein Globules in Charged Hydrogel Particles. Langmuir, 2017, 33, 4567-4577.	3.5	21
61	Interaction of Charged Patchy Protein Models with Like-Charged Polyelectrolyte Brushes. Langmuir, 2017, 33, 417-427.	3.5	44
62	Principles for Tuning Hydrophobic Ligandâ€“Receptor Binding Kinetics. Journal of Chemical Theory and Computation, 2017, 13, 3012-3019.	5.3	13
63	Charged Dendrimers Revisited: Effective Charge and Surface Potential of Dendritic Polyglycerol Sulfate. Macromolecules, 2017, 50, 4759-4769.	4.8	32
64	Guanidinium can both Cause and Prevent the Hydrophobic Collapse of Biomacromolecules. Journal of the American Chemical Society, 2017, 139, 863-870.	13.7	76
65	Catalyzed Bimolecular Reactions in Responsive Nanoreactors. ACS Catalysis, 2017, 7, 5604-5611.	11.2	53
66	Cosolute Partitioning in Polymer Networks: Effects of Flexibility and Volume Transitions. Macromolecules, 2017, 50, 6227-6237.	4.8	27
67	Temperature-Dependent Implicit-Solvent Model of Polyethylene Glycol in Aqueous Solution. Journal of Chemical Theory and Computation, 2017, 13, 6317-6327.	5.3	22
68	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
69	Stochastic level-set variational implicit-solvent approach to solute-solvent interfacial fluctuations. Journal of Chemical Physics, 2016, 145, 054114.	3.0	10
70	Communication: Resonance reaction in diffusion-influenced bimolecular reactions. Journal of Chemical Physics, 2016, 144, 081102.	3.0	3
71	Potential of mean force and transient states in polyelectrolyte pair complexation. Journal of Chemical Physics, 2016, 145, 034901.	3.0	16
72	Thermosensitive Cu‹sub›2‹/sub›Oâ€“PNIPAM coreâ€“shell nanoreactors with tunable photocatalytic activity. Journal of Materials Chemistry A, 2016, 4, 9677-9684.	10.3	46

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73	Confined Water Determines Transport Properties of Guest Molecules in Narrow Pores. ACS Nano, 2016, 10, 7646-7656.	14.6	66
74	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
75	Reaction rate of a composite coreâ€“shell nanoreactor with multiple nanocatalysts. Physical Chemistry Chemical Physics, 2016, 18, 20758-20767.	2.8	18
76	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
77	Solvent Fluctuations Induce Non-Markovian Kinetics in Hydrophobic Pocket-Ligand Binding. Journal of Physical Chemistry B, 2016, 120, 8127-8136.	2.6	8
78	Tuning the critical solution temperature of polymers by copolymerization. Journal of Chemical Physics, 2015, 143, 243119.	3.0	9
79	Theory of Solvation-Controlled Reactions in Stimuli-Responsive Nanoreactors. Journal of Physical Chemistry C, 2015, 119, 15723-15730.	3.1	37
80	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
81	Curvature Dependence of Hydrophobic Hydration Dynamics. Physical Review Letters, 2015, 114, 187802.	7.8	17
82	Interaction of human serum albumin with short polyelectrolytes: a study by calorimetry and computer simulations. Soft Matter, 2015, 11, 4630-4639.	2.7	64
83	LS-VISM: A software package for analysis of biomolecular solvation. Journal of Computational Chemistry, 2015, 36, 1047-1059.	3.3	18
84	Like-charged protein-polyelectrolyte complexation driven by charge patches. Journal of Chemical Physics, 2015, 143, 064905.	3.0	47
85	Charged patchy particle models in explicit salt: Ion distributions, electrostatic potentials, and effective interactions. Journal of Chemical Physics, 2015, 143, 064904.	3.0	38
86	Anisotropic Electrostatic Friction of para-Sexiphenyl on the ZnO (101Ì…0) Surface. Journal of Physical Chemistry C, 2014, 118, 26368-26376.	3.1	9
87	Dynamic density functional theory of protein adsorption on polymer-coated nanoparticles. Soft Matter, 2014, 10, 7932-7945.	2.7	37
88	Thermodynamic Description of Hofmeister Effects on the LCST of Thermosensitive Polymers. Journal of Physical Chemistry B, 2014, 118, 10979-10988.	2.6	93
89	Thermodynamic Description of the LCST of Charged Thermoresponsive Copolymers. Macromolecules, 2014, 47, 2096-2102.	4.8	47
90	Variational Implicit Solvation with Poissonâ€“Boltzmann Theory. Journal of Chemical Theory and Computation, 2014, 10, 1454-1467.	5.3	45

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91	Heterogeneous Hydration of p53/MDM2 Complex. Journal of Chemical Theory and Computation, 2014, 10, 1302-1313.	5.3	22
92	Protein Interactions with Polymer Coatings and Biomaterials. Angewandte Chemie - International Edition, 2014, 53, 8004-8031.	13.8	614
93	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
94	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
95	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
96	Rationalizing Polymer Swelling and Collapse under Attractive Cosolvent Conditions. Macromolecules, 2013, 46, 1231-1238.	4.8	88
97	Adsorption of proteins to functional polymeric nanoparticles. Polymer, 2013, 54, 2835-2849.	3.8	94
98	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
99	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
100	Catalysis by metallic nanoparticles in aqueous solution: model reactions. Chemical Society Reviews, 2012, 41, 5577.	38.1	966
101	Coreâ€“shell microgels as â€œsmartâ€•carriers for enzymes. Soft Matter, 2012, 8, 1428-1436.	2.7	103
102	Ion-specific counterion condensation on charged peptides: Poissonâ€“Boltzmann vs. atomistic simulations. Soft Matter, 2012, 8, 9338.	2.7	44
103	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
104	Effects of Hofmeister Ions on the Î±-Helical Structure of Proteins. Biophysical Journal, 2012, 102, 907-915.	0.5	46
105	Protein Sorption to Charged Microgels: Characterizing Binding Isotherms and Driving Forces. Langmuir, 2012, 28, 14373-14385.	3.5	76
106	Thermosensitive Auâ€PNIPA Yolkâ€“Shell Nanoparticles with Tunable Selectivity for Catalysis. Angewandte Chemie - International Edition, 2012, 51, 2229-2233.	13.8	350
107	How Interface Geometry Dictates Waterâ€™s Thermodynamic Signature in Hydrophobic Association. Journal of Statistical Physics, 2011, 145, 227-239.	1.2	10
108	Explicit and implicit modeling of nanobubbles in hydrophobic confinement. Anais Da Academia Brasileira De Ciencias, 2010, 82, 3-12.	0.8	12

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109	Electrolytes in a nanometer slab-confinement: Ion-specific structure and solvation forces. Journal of Chemical Physics, 2010, 133, 164511.	3.0	37
110	Ion-Specific Excluded-Volume Correlations and Solvation Forces. Physical Review Letters, 2010, 104, 097802.	7.8	42
111	Ion Specificity in Î±-Helical Folding Kinetics. Journal of Physical Chemistry B, 2010, 114, 13815-13822.	2.6	22
112	Molecular Insights into the Ion-Specific Kinetics of Anionic Peptides. Journal of Physical Chemistry B, 2010, 114, 7098-7103.	2.6	12
113	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
114	Structure-thermodynamics relation of electrolyte solutions. Journal of Chemical Physics, 2009, 130, 134507.	3.0	99
115	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
116	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
117	Ion-Specificity: From Solvation Thermodynamics to Molecular Simulations and Back. , 2009, , 231-265.		6
118	Sequence-Specific Size, Structure, and Stability of Tight Protein Knots. Biophysical Journal, 2009, 96, 831-839.	0.5	40
119	Salt-Specific Stability of Short and Charged Alanine-Based Î±-Helices. Journal of Physical Chemistry B, 2009, 113, 16689-16694.	2.6	21
120	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
121	Non-equilibrium sedimentation of colloids: confocal microscopy and Brownian dynamics simulations. Journal of Physics Condensed Matter, 2008, 20, 494222.	1.8	12
122	Application of the level-set method to the implicit solvation of nonpolar molecules. Journal of Chemical Physics, 2007, 127, 084503.	3.0	81
123	Interface dynamics of microscopic cavities in water. Journal of Chemical Physics, 2007, 126, 194504.	3.0	18