Jana Shen

List of Publications by Year
in descending order

121 papers	6,442 citations	53794 45 h-index	79698 73 g-index
133 all docs	133 docs citations	133 times ranked	5941 citing authors

#	Article	IF	Citations
1	Biofabrication with Chitosan. Biomacromolecules, 2005, 6, 2881-2894.	5.4	667
2	Voltage-Dependent Assembly of the Polysaccharide Chitosan onto an Electrode Surface. Langmuir, 2002, 18, 8620-8625.	3.5	283
3	Progress in the prediction of p<i>K</i>_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
4	Continuous Constant pH Molecular Dynamics in Explicit Solvent with pH-Based Replica Exchange. Journal of Chemical Theory and Computation, 2011, 7, 2617-2629.	5.3	182
5	In situ quantitative visualization and characterization of chitosan electrodeposition with paired sidewall electrodes. Soft Matter, 2010, 6, 3177.	2.7	150
6	Electroaddressing of Cell Populations by Coâ€Deposition with Calcium Alginate Hydrogels. Advanced Functional Materials, 2009, 19, 2074-2080.	14.9	115
7	Spatially Selective Deposition of a Reactive Polysaccharide Layer onto a Patterned Template. Langmuir, 2003, 19, 519-524.	3.5	111
8	Biomimetic Approach to Confer Redox Activity to Thin Chitosan Films. Advanced Functional Materials, 2010, 20, 2683-2694.	14.9	109
9	Mechanism of anodic electrodeposition of calcium alginate. Soft Matter, 2011, 7, 5677.	2.7	103
10	Recent development and application of constant pH molecular dynamics. Molecular Simulation, 2014, 40, 830-838.	2.0	102
11	All-Atom Continuous Constant pH Molecular Dynamics With Particle Mesh Ewald and Titratable Water. Journal of Chemical Theory and Computation, 2016, 12, 5411-5421.	5.3	101
12	Biofabrication to build the biologyâ€“device interface. Biofabrication, 2010, 2, 022002.	7.1	94
13	Mechanism of pH-dependent activation of the sodium-proton antiporter NhaA. Nature Communications, 2016, 7, 12940.	12.8	90
14	pH-Responsive Self-Assembly of Polysaccharide through a Rugged Energy Landscape. Journal of the American Chemical Society, 2015, 137, 13024-13030.	13.7	89
15	Chitosan to Connect Biology to Electronics: Fabricating the Bio-Device Interface and Communicating Across This Interface. Polymers, 2015, 7, 1-46.	4.5	87
16	Charge-leveling and proper treatment of long-range electrostatics in all-atom molecular dynamics at constant pH. Journal of Chemical Physics, 2012, 137, 184105.	3.0	86
17	Amplified and in Situ Detection of Redox-Active Metabolite Using a Biobased Redox Capacitor. Analytical Chemistry, 2013, 85, 2102-2108.	6.5	86
18	Electrodeposition of a Biopolymeric Hydrogel: Potential for One-Step Protein Electroaddressing. Biomacromolecules, 2012, 13, 1181-1189.	5.4	82

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19	Assessing Lysine and Cysteine Reactivities for Designing Targeted Covalent Kinase Inhibitors. Journal of the American Chemical Society, 2019, 141, 6553-6560.	13.7	80
20	Predicting pKa Values with Continuous Constant pH Molecular Dynamics. Methods in Enzymology, 2009, 466, 455-475.	1.0	77
21	Biofabrication: programmable assembly of polysaccharide hydrogels in microfluidics as biocompatible scaffolds. Journal of Materials Chemistry, 2012, 22, 7659.	6.7	75
22	Introducing Titratable Water to All-Atom Molecular Dynamics at ConstantÂpH. Biophysical Journal, 2013, 105, L15-L17.	0.5	72
23	pH-Dependent Population Shift Regulates BACE1 Activity and Inhibition. Journal of the American Chemical Society, 2015, 137, 9543-9546.	13.7	72
24	Redox-capacitor to connect electrochemistry to redox-biology. Analyst, The, 2014, 139, 32-43.	3.5	71
25	Chitosan-mediated in situ biomolecule assembly in completely packaged microfluidic devices. Lab on A Chip, 2006, 6, 1315.	6.0	68
26	Reverse Engineering Applied to Red Human Hair Pheomelanin Reveals Redox-Buffering as a Pro-Oxidant Mechanism. Scientific Reports, 2015, 5, 18447.	3.3	67
27	Coding for hydrogel organization through signal guided self-assembly. Soft Matter, 2014, 10, 465-469.	2.7	66
28	Redox Capacitor to Establish Bioâ€Device Redoxâ€Connectivity. Advanced Functional Materials, 2012, 22, 1409-1416.	14.9	65
29	A Robust Technique for Assembly of Nucleic Acid Hybridization Chips Based on Electrochemically Templated Chitosan. Analytical Chemistry, 2004, 76, 365-372.	6.5	61
30	Electroaddressing Functionalized Polysaccharides as Model Biofilms for Interrogating Cell Signaling. Advanced Functional Materials, 2012, 22, 519-528.	14.9	61
31	Electrodeposition of a weak polyelectrolyte hydrogel: remarkable effects of salt on kinetics, structure and properties. Soft Matter, 2013, 9, 2703.	2.7	59
32	Programmable Electrofabrication of Porous Janus Films with Tunable Janus Balance for Anisotropic Cell Guidance and Tissue Regeneration. Advanced Functional Materials, 2019, 29, 1900065.	14.9	58
33	Proton-Coupled Conformational Activation of SARS Coronavirus Main Proteases and Opportunity for Designing Small-Molecule Broad-Spectrum Targeted Covalent Inhibitors. Journal of the American Chemical Society, 2020, 142, 21883-21890.	13.7	57
34	How Î¼-opioid receptor recognizes fentanyl. Nature Communications, 2021, 12, 984.	12.8	56
35	Toward accurate prediction of p<i>K</i>_a values for internal protein residues: The importance of conformational relaxation and desolvation energy. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3364-3373.	2.6	54
36	Biofabricating Multifunctional Soft Matter with Enzymes and Stimuliâ€Responsive Materials. Advanced Functional Materials, 2012, 22, 3004-3012.	14.9	54

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37	Constant pH Molecular Dynamics Reveals How Proton Release Drives the Conformational Transition of a Transmembrane Efflux Pump. Journal of Chemical Theory and Computation, 2017, 13, 6405-6414.	5.3	54
38	Redox-Cycling and H₂O₂ Generation by Fabricated Catecholic Films in the Absence of Enzymes. Biomacromolecules, 2011, 12, 880-888.	5.4	53
39	Electronic modulation of biochemical signal generation. Nature Nanotechnology, 2014, 9, 605-610.	31.5	52
40	Mechanism of the pH-Controlled Self-Assembly of Nanofibers from Peptide Amphiphiles. Journal of Physical Chemistry C, 2014, 118, 16272-16278.	3.1	52
41	Conformational Activation of a Transmembrane Proton Channel from Constant pH Molecular Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 3961-3966.	4.6	52
42	Biomimetic fabrication of information-rich phenolic-chitosan films. Soft Matter, 2011, 7, 9601.	2.7	51
43	Biospecific Selfâ€Assembly of a Nanoparticle Coating for Targeted and Stimuliâ€Responsive Drug Delivery. Advanced Functional Materials, 2015, 25, 1404-1417.	14.9	50
44	Electro-molecular Assembly: Electrical Writing of Information into an Erasable Polysaccharide Medium. ACS Applied Materials & Interfaces, 2016, 8, 19780-19786.	8.0	49
45	Constant pH Molecular Dynamics Reveals pH-Modulated Binding of Two Small-Molecule BACE1 Inhibitors. Journal of Physical Chemistry Letters, 2016, 7, 944-949.	4.6	48
46	Generalized Born Based Continuous Constant pH Molecular Dynamics in Amber: Implementation, Benchmarking and Analysis. Journal of Chemical Information and Modeling, 2018, 58, 1372-1383.	5.4	48
47	Compartmentalized Multilayer Hydrogel Formation Using a Stimulus-Responsive Self-Assembling Polysaccharide. ACS Applied Materials & Interfaces, 2014, 6, 2948-2957.	8.0	47
48	Reversible Programing of Soft Matter with Reconfigurable Mechanical Properties. Advanced Functional Materials, 2017, 27, 1605665.	14.9	46
49	Redox Probing for Chemical Information of Oxidative Stress. Analytical Chemistry, 2017, 89, 1583-1592.	6.5	46
50	Electrical Programming of Soft Matter: Using Temporally Varying Electrical Inputs To Spatially Control Self Assembly. Biomacromolecules, 2018, 19, 364-373.	5.4	46
51	GPU-Accelerated Implementation of Continuous Constant pH Molecular Dynamics in Amber: p<i>K</i>_a Predictions with Single-pH Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4821-4832.	5.4	46
52	Assessment of proton-coupled conformational dynamics of SARS and MERS coronavirus papain-like proteases: Implication for designing broad-spectrum antiviral inhibitors. Journal of Chemical Physics, 2020, 153, 115101.	3.0	46
53	Atomistic simulations of pH-dependent self-assembly of micelle and bilayer from fatty acids. Journal of Chemical Physics, 2012, 137, 194902.	3.0	45
54	Thermodynamic Coupling of Protonation and Conformational Equilibria in Proteins: Theory and Simulation. Biophysical Journal, 2012, 102, 1590-1597.	0.5	45

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55	Reverse Engineering To Suggest Biologically Relevant Redox Activities of Phenolic Materials. ACS Chemical Biology, 2013, 8, 716-724.	3.4	44
56	Electrochemical Measurement of the Î²-Galactosidase Reporter from Live Cells: A Comparison to the Miller Assay. ACS Synthetic Biology, 2016, 5, 28-35.	3.8	44
57	Using a Redox Modality to Connect Synthetic Biology to Electronics: Hydrogelâ€Based Chemoâ€Electro Signal Transduction for Molecular Communication. Advanced Healthcare Materials, 2017, 6, 1600908.	7.6	44
58	Reagentless Protein Assembly Triggered by Localized Electrical Signals. Advanced Materials, 2009, 21, 984-988.	21.0	43
59	Unraveling a Trap-and-Trigger Mechanism in the pH-Sensitive Self-Assembly of Spider Silk Proteins. Journal of Physical Chemistry Letters, 2012, 3, 658-662.	4.6	43
60	Electrobiofabrication: electrically based fabrication with biologically derived materials. Biofabrication, 2019, 11, 032002.	7.1	43
61	Reversible Electroaddressing of Selfâ€assembling Aminoâ€Acid Conjugates. Advanced Functional Materials, 2011, 21, 1575-1580.	14.9	42
62	Self-Assembly and Bilayerâ€“Micelle Transition of Fatty Acids Studied by Replica-Exchange Constant pH Molecular Dynamics. Langmuir, 2013, 29, 14823-14830.	3.5	42
63	Connecting Biology to Electronics: Molecular Communication via Redox Modality. Advanced Healthcare Materials, 2017, 6, 1700789.	7.6	40
64	Redox Is a Global Biodevice Information Processing Modality. Proceedings of the IEEE, 2019, 107, 1402-1424.	21.3	37
65	Inâ€Film Bioprocessing and Immunoanalysis with Electroaddressable Stimuliâ€Responsive Polysaccharides. Advanced Functional Materials, 2010, 20, 1645-1652.	14.9	36
66	Redox cycling-based amplifying electrochemical sensor for in situ clozapine antipsychotic treatment monitoring. Electrochimica Acta, 2014, 130, 497-503.	5.2	36
67	Reverse Engineering To Characterize Redox Properties: Revealing Melaninâ€™s Redox Activity through Mediated Electrochemical Probing. Chemistry of Materials, 2018, 30, 5814-5826.	6.7	36
68	Toward Understanding the Environmental Control of Hydrogel Film Properties: How Salt Modulates the Flexibility of Chitosan Chains. Macromolecules, 2017, 50, 5946-5952.	4.8	35
69	Predicting Catalytic Proton Donors and Nucleophiles in Enzymes: How Adding Dynamics Helps Elucidate the Structureâ€“Function Relationships. Journal of Physical Chemistry Letters, 2018, 9, 1179-1184.	4.6	35
70	Diarylcyclopentendione Metabolite Obtained from a <i>Preussia typharum</i> Isolate Procured Using an Unconventional Cultivation Approach. Journal of Natural Products, 2012, 75, 1819-1823.	3.0	33
71	Information processing through a bio-based redox capacitor: Signatures for redox-cycling. Bioelectrochemistry, 2014, 98, 94-102.	4.6	33
72	Nano-guided cell networks as conveyors of molecular communication. Nature Communications, 2015, 6, 8500.	12.8	33

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73	Electrochemical reverse engineering: A systems-level tool to probe the redox-based molecular communication of biology. Free Radical Biology and Medicine, 2017, 105, 110-131.	2.9	32
74	Proton-Coupled Conformational Allostery Modulates the Inhibitor Selectivity for Î²-Secretase. Journal of Physical Chemistry Letters, 2017, 8, 4832-4837.	4.6	32
75	Electrochemical Study of the Catechol-Modified Chitosan System for Clozapine Treatment Monitoring. Langmuir, 2014, 30, 14686-14693.	3.5	31
76	Electrochemical Fabrication of Functional Gelatin-Based Bioelectronic Interface. Biomacromolecules, 2016, 17, 558-563.	5.4	31
77	Accessing biology's toolbox for the mesoscale biofabrication of soft matter. Soft Matter, 2013, 9, 6019.	2.7	30
78	Electrofabrication of functional materials: Chloramine-based antimicrobial film for infectious wound treatment. Acta Biomaterialia, 2018, 73, 190-203.	8.3	30
79	How Electrostatic Coupling Enables Conformational Plasticity in a Tyrosine Kinase. Journal of the American Chemical Society, 2019, 141, 15092-15101.	13.7	30
80	Predicting Reactive Cysteines with Implicit-Solvent-Based Continuous Constant pH Molecular Dynamics in Amber. Journal of Chemical Theory and Computation, 2020, 16, 3689-3698.	5.3	30
81	How Ligand Protonation State Controls Water in Proteinâ€“Ligand Binding. Journal of Physical Chemistry Letters, 2018, 9, 5440-5444.	4.6	29
82	Uncovering Specific Electrostatic Interactions in the Denatured States of Proteins. Biophysical Journal, 2010, 99, 924-932.	0.5	28
83	Electroaddressing Agarose Using Fmoc-Phenylalanine as a Temporary Scaffold. Langmuir, 2011, 27, 7380-7384.	3.5	28
84	Electrochemical Probing through a Redox Capacitor To Acquire Chemical Information on Biothiols. Analytical Chemistry, 2016, 88, 7213-7221.	6.5	27
85	Electrical Writing onto a Dynamically Responsive Polysaccharide Medium: Patterning Structure and Function into a Reconfigurable Medium. Advanced Functional Materials, 2018, 28, 1803139.	14.9	27
86	Simulating pH Titration of a Single Surfactant in Ionic and Nonionic Surfactant Micelles. Journal of Physical Chemistry B, 2011, 115, 14980-14990.	2.6	25
87	Alternative proton-binding site and long-distance coupling in <i>Escherichia coli</i> sodiumâ€“proton antiporter NhaA. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 25517-25522.	7.1	25
88	Hierarchical patterning via dynamic sacrificial printing of stimuli-responsive hydrogels. Biofabrication, 2020, 12, 035007.	7.1	25
89	Conformational dynamics of cathepsin D and binding to a smallâ€molecule BACE1 inhibitor. Journal of Computational Chemistry, 2017, 38, 1260-1269.	3.3	24
90	Programmable â€œSemismartâ€•Sensor: Relevance to Monitoring Antipsychotics. Advanced Functional Materials, 2015, 25, 2156-2165.	14.9	23

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91	Catechol-Based Hydrogel for Chemical Information Processing. Biomimetics, 2017, 2, 11.	3.3	21
92	Kinetics and Mechanism of Fentanyl Dissociation from the Î¼-Opioid Receptor. Jacs Au, 2021, 1, 2208-2215.	7.9	21
93	Exploring pH-Responsive, Switchable Crosslinking Mechanisms for Programming Reconfigurable Hydrogels Based on Aminopolysaccharides. Chemistry of Materials, 2018, 30, 8597-8605.	6.7	19
94	Electronic structure properties of solvated biomolecules: A quantum approach for macromolecular characterization. Journal of Computational Chemistry, 2000, 21, 1562-1571.	3.3	18
95	Ligand-induced allostery in the interaction of the <i>Pseudomonas aeruginosa</i> heme binding protein with heme oxygenase. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3421-3426.	7.1	18
96	Reactivities of the Front Pocket N-Terminal Cap Cysteines in Human Kinases. Journal of Medicinal Chemistry, 2022, 65, 1525-1535.	6.4	18
97	Enzymatic Writing to Soft Films: Potential to Filter, Store, and Analyze Biologically Relevant Chemical Information. Advanced Functional Materials, 2014, 24, 480-491.	14.9	17
98	An Electrochemical Micro-System for Clozapine Antipsychotic Treatment Monitoring. Electrochimica Acta, 2015, 163, 260-270.	5.2	17
99	Mediated Electrochemistry to Mimic Biology's Oxidative Assembly of Functional Matrices. Advanced Functional Materials, 2020, 30, 2001776.	14.9	17
100	Molecular dynamics simulations of ionic and nonionic surfactant micelles with a generalized born implicitâ€solvent model. Journal of Computational Chemistry, 2011, 32, 2348-2358.	3.3	16
101	Conformational Dynamics of Two Natively Unfolded Fragment Peptides: Comparison of the AMBER and CHARMM Force Fields. Journal of Physical Chemistry B, 2015, 119, 7902-7910.	2.6	16
102	Fusing Sensor Paradigms to Acquire Chemical Information: An Integrative Role for Smart Biopolymeric Hydrogels. Advanced Healthcare Materials, 2016, 5, 2595-2616.	7.6	16
103	Electrochemistry for bio-device molecular communication: The potential to characterize, analyze and actuate biological systems. Nano Communication Networks, 2017, 11, 76-89.	2.9	15
104	Catechol-chitosan redox capacitor for added amplification in electrochemical immunoanalysis. Colloids and Surfaces B: Biointerfaces, 2018, 169, 470-477.	5.0	15
105	Electrical cuing of chitosan's mesoscale organization. Reactive and Functional Polymers, 2020, 148, 104492.	4.1	15
106	Coupling Self-Assembly Mechanisms to Fabricate Molecularly and Electrically Responsive Films. Biomacromolecules, 2019, 20, 969-978.	5.4	14
107	A Method To Determine Residue-Specific Unfolded-State p<i>K</i>_a Values from Analysis of Stability Changes in Single Mutant Cycles. Journal of the American Chemical Society, 2010, 132, 7258-7259.	13.7	13
108	Biofabricated Nanoparticle Coating for Liverâ€Cell Targeting. Advanced Healthcare Materials, 2015, 4, 1972-1981.	7.6	13

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109	Effects of system net charge and electrostatic truncation on all-atom constant pH molecular dynamics. Journal of Computational Chemistry, 2014, 35, 1986-1996.	3.3	12
110	Reversibly Reconfigurable Cross-Linking Induces Fusion of Separate Chitosan Hydrogel Films. ACS Applied Bio Materials, 2018, 1, 1695-1704.	4.6	12
111	Continuous Constant pH Molecular Dynamics Simulations of Transmembrane Proteins. Methods in Molecular Biology, 2021, 2302, 275-287.	0.9	11
112	Polyelectrolyte in Electric Field: Disparate Conformational Behavior along an Aminopolysaccharide Chain. ACS Omega, 2020, 5, 12016-12026.	3.5	11
113	Multidimensional Mapping Method Using an Arrayed Sensing System for Cross-Reactivity Screening. PLoS ONE, 2015, 10, e0116310.	2.5	10
114	pH-Dependent cooperativity and existence of a dry molten globule in the folding of a miniprotein BBL. Physical Chemistry Chemical Physics, 2018, 20, 3523-3530.	2.8	10
115	Profiling MAP kinase cysteines for targeted covalent inhibitor design. RSC Medicinal Chemistry, 2022, 13, 54-63.	3.9	10
116	Exploring the pH-Dependent Structureâ€"Dynamicsâ€"Function Relationship of Human Renin. Journal of Chemical Information and Modeling, 2021, 61, 400-407.	5.4	8
117	Exploring the pH- and Ligand-Dependent Flap Dynamics of Malarial Plasmepsin II. Journal of Chemical Information and Modeling, 2022, 62, 150-158.	5.4	8
118	Catechol Patterned Film Enables the Enzymatic Detection of Glucose with Cell Phone Imaging. ACS Sustainable Chemistry and Engineering, 2021, 9, 14836-14845.	6.7	7
119	Nascent Î² -Hairpin Formation of a Natively Unfolded Peptide Reveals the Role of Hydrophobic Contacts. Biophysical Journal, 2015, 109, 630-638.	0.5	6
120	Nucleotide Dynamics at the A-Site Cleft in the Peptidyltransferase Center of <i>H. marismortui</i> 50S Ribosomal Subunits. Journal of Physical Chemistry Letters, 2012, 3, 1007-1010.	4.6	5
121	Zooming in on a small multidrug transporter reveals details of asymmetric protonation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8060-8062.	7.1	2