Jana Shen

List of Publications by Year
in descending order

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Version: 2024-02-01

121	6,442	53794 45	79698 73
papers	citations	h-index	g-index

133	133	133	5941
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reactivities of the Front Pocket N-Terminal Cap Cysteines in Human Kinases. Journal of Medicinal Chemistry, 2022, 65, 1525-1535.	6.4	18
2	Profiling MAP kinase cysteines for targeted covalent inhibitor design. RSC Medicinal Chemistry, 2022, 13, 54-63.	3.9	10
3	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
4	Continuous Constant pH Molecular Dynamics Simulations of Transmembrane Proteins. Methods in Molecular Biology, 2021, 2302, 275-287.	0.9	11
5	How Î¼-opioid receptor recognizes fentanyl. Nature Communications, 2021, 12, 984.	12.8	56
6	Exploring the pH-Dependent Structureâ€“Dynamicsâ€“Function Relationship of Human Renin. Journal of Chemical Information and Modeling, 2021, 61, 400-407.	5.4	8
7	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
8	Kinetics and Mechanism of Fentanyl Dissociation from the Î¼-Opioid Receptor. Jacs Au, 2021, 1, 2208-2215.	7.9	21
9	Alternative proton-binding site and long-distance coupling in Escherichia coli sodiumâ€“proton antiporter NhaA. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 25517-25522.	7.1	25
10	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
11	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
12	Mediated Electrochemistry to Mimic Biology's Oxidative Assembly of Functional Matrices. Advanced Functional Materials, 2020, 30, 2001776.	14.9	17
13	Hierarchical patterning via dynamic sacrificial printing of stimuli-responsive hydrogels. Biofabrication, 2020, 12, 035007.	7.1	25
14	Electrical cuing of chitosan's mesoscale organization. Reactive and Functional Polymers, 2020, 148, 104492.	4.1	15
15	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
16	Polyelectrolyte in Electric Field: Disparate Conformational Behavior along an Aminopolysaccharide Chain. ACS Omega, 2020, 5, 12016-12026.	3.5	11
17	GPU-Accelerated Implementation of Continuous Constant pH Molecular Dynamics in Amber: pK_a Predictions with Single-pH Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4821-4832.	5.4	46
18	How Electrostatic Coupling Enables Conformational Plasticity in a Tyrosine Kinase. Journal of the American Chemical Society, 2019, 141, 15092-15101.	13.7	30

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19	Redox Is a Global Biodevice Information Processing Modality. Proceedings of the IEEE, 2019, 107, 1402-1424.	21.3	37
20	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
21	Assessing Lysine and Cysteine Reactivities for Designing Targeted Covalent Kinase Inhibitors. Journal of the American Chemical Society, 2019, 141, 6553-6560.	13.7	80
22	Electrobiofabrication: electrically based fabrication with biologically derived materials. Biofabrication, 2019, 11, 032002.	7.1	43
23	Coupling Self-Assembly Mechanisms to Fabricate Molecularly and Electrically Responsive Films. Biomacromolecules, 2019, 20, 969-978.	5.4	14
24	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
25	Electrofabrication of functional materials: Chloramine-based antimicrobial film for infectious wound treatment. Acta Biomaterialia, 2018, 73, 190-203.	8.3	30
26	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
27	Electrical Programming of Soft Matter: Using Temporally Varying Electrical Inputs To Spatially Control Self Assembly. Biomacromolecules, 2018, 19, 364-373.	5.4	46
28	Exploring pH-Responsive, Switchable Crosslinking Mechanisms for Programming Reconfigurable Hydrogels Based on Aminopolysaccharides. Chemistry of Materials, 2018, 30, 8597-8605.	6.7	19
29	Reversibly Reconfigurable Cross-Linking Induces Fusion of Separate Chitosan Hydrogel Films. ACS Applied Bio Materials, 2018, 1, 1695-1704.	4.6	12
30	How Ligand Protonation State Controls Water in Proteinâ€“Ligand Binding. Journal of Physical Chemistry Letters, 2018, 9, 5440-5444.	4.6	29
31	Catechol-chitosan redox capacitor for added amplification in electrochemical immunoanalysis. Colloids and Surfaces B: Biointerfaces, 2018, 169, 470-477.	5.0	15
32	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
33	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
34	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
35	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
36	Reversible Programing of Soft Matter with Reconfigurable Mechanical Properties. Advanced Functional Materials, 2017, 27, 1605665.	14.9	46

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37	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
38	Conformational dynamics of cathepsin D and binding to a smallâ€molecule BACE1 inhibitor. Journal of Computational Chemistry, 2017, 38, 1260-1269.	3.3	24
39	Ligand-induced allostery in the interaction of the Pseudomonas aeruginosa 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
40	Redox Probing for Chemical Information of Oxidative Stress. Analytical Chemistry, 2017, 89, 1583-1592.	6.5	46
41	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
42	Connecting Biology to Electronics: Molecular Communication via Redox Modality. Advanced Healthcare Materials, 2017, 6, 1700789.	7.6	40
43	Proton-Coupled Conformational Allostery Modulates the Inhibitor Selectivity for Î²-Secretase. Journal of Physical Chemistry Letters, 2017, 8, 4832-4837.	4.6	32
44	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
45	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
46	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
47	Catechol-Based Hydrogel for Chemical Information Processing. Biomimetics, 2017, 2, 11.	3.3	21
48	Electrochemical Probing through a Redox Capacitor To Acquire Chemical Information on Biothiols. Analytical Chemistry, 2016, 88, 7213-7221.	6.5	27
49	Mechanism of pH-dependent activation of the sodium-proton antiporter NhaA. Nature Communications, 2016, 7, 12940.	12.8	90
50	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
51	Fusing Sensor Paradigms to Acquire Chemical Information: An Integrative Role for Smart Biopolymeric Hydrogels. Advanced Healthcare Materials, 2016, 5, 2595-2616.	7.6	16
52	Conformational Activation of a Transmembrane Proton Channel from Constant pH Molecular Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 3961-3966.	4.6	52
53	Electro-molecular Assembly: Electrical Writing of Information into an Erasable Polysaccharide Medium. ACS Applied Materials & Interfaces, 2016, 8, 19780-19786.	8.0	49
54	Electrochemical Fabrication of Functional Gelatin-Based Bioelectronic Interface. Biomacromolecules, 2016, 17, 558-563.	5.4	31

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55	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
56	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
57	Reverse Engineering Applied to Red Human Hair Pheomelanin Reveals Redox-Buffering as a Pro-Oxidant Mechanism. Scientific Reports, 2015, 5, 18447.	3.3	67
58	Biofabricated Nanoparticle Coating for Liverâ€Cell Targeting. Advanced Healthcare Materials, 2015, 4, 1972-1981.	7.6	13
59	Programmable â€œSemismartâ€•Sensor: Relevance to Monitoring Antipsychotics. Advanced Functional Materials, 2015, 25, 2156-2165.	14.9	23
60	Multidimensional Mapping Method Using an Arrayed Sensing System for Cross-Reactivity Screening. PLoS ONE, 2015, 10, e0116310.	2.5	10
61	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
62	Biospecific Selfâ€Assembly of a Nanoparticle Coating for Targeted and Stimuliâ€Responsive Drug Delivery. Advanced Functional Materials, 2015, 25, 1404-1417.	14.9	50
63	An Electrochemical Micro-System for Clozapine Antipsychotic Treatment Monitoring. Electrochimica Acta, 2015, 163, 260-270.	5.2	17
64	Nascent Î² -Hairpin Formation of a Natively Unfolded Peptide Reveals the Role of Hydrophobic Contacts. Biophysical Journal, 2015, 109, 630-638.	0.5	6
65	Chitosan to Connect Biology to Electronics: Fabricating the Bio-Device Interface and Communicating Across This Interface. Polymers, 2015, 7, 1-46.	4.5	87
66	pH-Dependent Population Shift Regulates BACE1 Activity and Inhibition. Journal of the American Chemical Society, 2015, 137, 9543-9546.	13.7	72
67	Nano-guided cell networks as conveyors of molecular communication. Nature Communications, 2015, 6, 8500.	12.8	33
68	pH-Responsive Self-Assembly of Polysaccharide through a Rugged Energy Landscape. Journal of the American Chemical Society, 2015, 137, 13024-13030.	13.7	89
69	Electrochemical Study of the Catechol-Modified Chitosan System for Clozapine Treatment Monitoring. Langmuir, 2014, 30, 14686-14693.	3.5	31
70	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
71	Information processing through a bio-based redox capacitor: Signatures for redox-cycling. Bioelectrochemistry, 2014, 98, 94-102.	4.6	33
72	Redox cycling-based amplifying electrochemical sensor for in situ clozapine antipsychotic treatment monitoring. Electrochimica Acta, 2014, 130, 497-503.	5.2	36

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73	Redox-capacitor to connect electrochemistry to redox-biology. Analyst, The, 2014, 139, 32-43.	3.5	71
74	Coding for hydrogel organization through signal guided self-assembly. Soft Matter, 2014, 10, 465-469.	2.7	66
75	Electronic modulation of biochemical signal generation. Nature Nanotechnology, 2014, 9, 605-610.	31.5	52
76	Compartmentalized Multilayer Hydrogel Formation Using a Stimulus-Responsive Self-Assembling Polysaccharide. ACS Applied Materials & Interfaces, 2014, 6, 2948-2957.	8.0	47
77	Mechanism of the pH-Controlled Self-Assembly of Nanofibers from Peptide Amphiphiles. Journal of Physical Chemistry C, 2014, 118, 16272-16278.	3.1	52
78	Recent development and application of constant pH molecular dynamics. Molecular Simulation, 2014, 40, 830-838.	2.0	102
79	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
80	Amplified and in Situ Detection of Redox-Active Metabolite Using a Biobased Redox Capacitor. Analytical Chemistry, 2013, 85, 2102-2108.	6.5	86
81	Introducing Titratable Water to All-Atom Molecular Dynamics at ConstantÂpH. Biophysical Journal, 2013, 105, L15-L17.	0.5	72
82	Electrodeposition of a weak polyelectrolyte hydrogel: remarkable effects of salt on kinetics, structure and properties. Soft Matter, 2013, 9, 2703.	2.7	59
83	Accessing biology's toolbox for the mesoscale biofabrication of soft matter. Soft Matter, 2013, 9, 6019.	2.7	30
84	Reverse Engineering To Suggest Biologically Relevant Redox Activities of Phenolic Materials. ACS Chemical Biology, 2013, 8, 716-724.	3.4	44
85	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
86	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
87	Atomistic simulations of pH-dependent self-assembly of micelle and bilayer from fatty acids. Journal of Chemical Physics, 2012, 137, 194902.	3.0	45
88	Electrodeposition of a Biopolymeric Hydrogel: Potential for One-Step Protein Electroaddressing. Biomacromolecules, 2012, 13, 1181-1189.	5.4	82
89	Nucleotide Dynamics at the A-Site Cleft in the Peptidyltransferase Center of H. marismortui 50S Ribosomal Subunits. Journal of Physical Chemistry Letters, 2012, 3, 1007-1010.	4.6	5
90	Diarylcyclopentendione Metabolite Obtained from a Preussia typharum Isolate Procured Using an Unconventional Cultivation Approach. Journal of Natural Products, 2012, 75, 1819-1823.	3.0	33

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91	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
92	Thermodynamic Coupling of Protonation and Conformational Equilibria in Proteins: Theory and Simulation. Biophysical Journal, 2012, 102, 1590-1597.	0.5	45
93	Biofabrication: programmable assembly of polysaccharide hydrogels in microfluidics as biocompatible scaffolds. Journal of Materials Chemistry, 2012, 22, 7659.	6.7	75
94	Redox Capacitor to Establish Bioâ€Device Redoxâ€Connectivity. Advanced Functional Materials, 2012, 22, 1409-1416.	14.9	65
95	Biofabricating Multifunctional Soft Matter with Enzymes and Stimuliâ€Responsive Materials. Advanced Functional Materials, 2012, 22, 3004-3012.	14.9	54
96	Electroaddressing Functionalized Polysaccharides as Model Biofilms for Interrogating Cell Signaling. Advanced Functional Materials, 2012, 22, 519-528.	14.9	61
97	Electroaddressing Agarose Using Fmoc-Phenylalanine as a Temporary Scaffold. Langmuir, 2011, 27, 7380-7384.	3.5	28
98	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
99	Redox-Cycling and H₂O₂ Generation by Fabricated Catecholic Films in the Absence of Enzymes. Biomacromolecules, 2011, 12, 880-888.	5.4	53
100	Mechanism of anodic electrodeposition of calcium alginate. Soft Matter, 2011, 7, 5677.	2.7	103
101	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
102	Biomimetic fabrication of information-rich phenolic-chitosan films. Soft Matter, 2011, 7, 9601.	2.7	51
103	Toward accurate prediction of pK_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
104	Progress in the prediction of pK_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
105	Reversible Electroaddressing of Selfâ€assembling Aminoâ€Acid Conjugates. Advanced Functional Materials, 2011, 21, 1575-1580.	14.9	42
106	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
107	Inâ€Film Bioprocessing and Immunoanalysis with Electroaddressable Stimuliâ€Responsive Polysaccharides. Advanced Functional Materials, 2010, 20, 1645-1652.	14.9	36
108	Biomimetic Approach to Confer Redox Activity to Thin Chitosan Films. Advanced Functional Materials, 2010, 20, 2683-2694.	14.9	109

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109	Biofabrication to build the biologyâ€“device interface. Biofabrication, 2010, 2, 022002.	7.1	94
110	Uncovering Specific Electrostatic Interactions in the Denatured States of Proteins. Biophysical Journal, 2010, 99, 924-932.	0.5	28
111	A Method To Determine Residue-Specific Unfolded-State pK_a Values from Analysis of Stability Changes in Single Mutant Cycles. Journal of the American Chemical Society, 2010, 132, 7258-7259.	13.7	13
112	In situ quantitative visualization and characterization of chitosan electrodeposition with paired sidewall electrodes. Soft Matter, 2010, 6, 3177.	2.7	150
113	Electroaddressing of Cell Populations by Coâ€Ðeposition with Calcium Alginate Hydrogels. Advanced Functional Materials, 2009, 19, 2074-2080.	14.9	115
114	Reagentless Protein Assembly Triggered by Localized Electrical Signals. Advanced Materials, 2009, 21, 984-988.	21.0	43
115	Predicting pKa Values with Continuous Constant pH Molecular Dynamics. Methods in Enzymology, 2009, 466, 455-475.	1.0	77
116	Chitosan-mediated in situ biomolecule assembly in completely packaged microfluidic devices. Lab on A Chip, 2006, 6, 1315.	6.0	68
117	Biofabrication with Chitosan. Biomacromolecules, 2005, 6, 2881-2894.	5.4	667
118	A Robust Technique for Assembly of Nucleic Acid Hybridization Chips Based on Electrochemically Templated Chitosan. Analytical Chemistry, 2004, 76, 365-372.	6.5	61
119	Spatially Selective Deposition of a Reactive Polysaccharide Layer onto a Patterned Template. Langmuir, 2003, 19, 519-524.	3.5	111
120	Voltage-Dependent Assembly of the Polysaccharide Chitosan onto an Electrode Surface. Langmuir, 2002, 18, 8620-8625.	3.5	283
121	Electronic structure properties of solvated biomolecules: A quantum approach for macromolecular characterization. Journal of Computational Chemistry, 2000, 21, 1562-1571.	3.3	18